(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property Organization
International Bureau



TERRETARIO DE CONTROL D

(43) International Publication Date 27 December 2002 (27.12.2002)

PCT

(10) International Publication Number WO 02/102974 A2

(51) International Patent Classification7:

- (21) International Application Number: PCT/US01/47994
- (22) International Filing Date:

10 December 2001 (10.12.2001)

(25) Filing Language:

English

C12N

(26) Publication Language:

English

(30) Priority Data:

60/254,353 60/301,878 8 December 2000 (08.12.2000) US 29 June 2001 (29.06.2001) US

- (71) Applicant: MEDIMMUNE, INC. [US/US]; 35 West Watkins Mill Road, Gaithersburg, MD 20878 (US).
- (72) Inventors: LANGERMANN, Solomon, R.; 6606 Cross Country Boulevard, Baltimore, MD 20878 (US). HULT-GREN, Scott, J.; 1068 Polo Downs, Town and Country, MO 63017 (US). HUNG, Chia-Suei; 1425 Cutter Avenue, St. Louis, MO 63139 (US). BOUCKAERT, Julie; 7549 Trenton Avenue, St. Louis, MO 63130 (US).
- (74) Agents: POISSANT, Brian, M. et al.; Pennie & Edmonds LLP, 1155 Avenue of the Americas, New York, NY 10036 (US).

- (81) Designated States (national): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW.
- (84) Designated States (regional): ARIPO patent (GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian patent (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM), European patent (AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR), OAPI patent (BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG).

Published:

 without international search report and to be republished upon receipt of that report

For two-letter codes and other abbreviations, refer to the "Guidance Notes on Codes and Abbreviations" appearing at the beginning of each regular issue of the PCT Gazette.

(54) Title: MUTANT PROTEINS, HIGH POTENCY INHIBITORY ANTIBODIES AND FIMCH CRYSTAL STRUCTURE

(57) Abstract: The present invention provides bacterial immunogenic agents for administration to humans and non-human animals to stimulate an immune response, It particularly relates to the vaccination of mammalian species, especially human patients, with variants of the Ecoli FimCH protein that elicit antibodies that have better functional inhibitory activity than antibodies raised against wild type protein. In particular, such variants include mutations that promote a more open confirmation of the FimH protein, particularly in regions involved in mannose binding, to expose regions previously poorly exposed and mutations that abolish a significantly reduce mannose binding. In another aspect, the invention provides antibodies against such proteins and protein complexes that may be used in passive immunization to protect or treat pathogenic bacterial infections. The present invention also provides machine readable media embedded with the three-dimensional atomic structure coordinates of FimCH bound to mannose, and subsets thereof, and methods of using the crystal structure to provide candidate amino acid residues for mutation.

ATTORNEY DOCKET NUMBER: 10271-112-999 SERIAL NUMBER: 10/823,253

REFERENCE: **B07**



MUTANT PROTEINS, HIGH POTENCY INHIBITORY ANTIBODIES AND FIMCH CRYSTAL STRUCTURE

This application claims priority to U.S. Provisional Patent Application No. 60/254,353, filed December 8, 2000, and U.S. Provisional Patent Application No. 60/301,878, filed June 29, 2001, the content of each of which is incorporated herein by reference in its entirety.

1. FIELD OF THE INVENTION

10 The invention relates to methods of producing antibodies, preferably antibodies that inhibit binding of a protein to its binding partner. Further, the methods include producing antibodies having enhanced functional inhibitory activity against a protein, for example, that inhibit binding of the protein to a binding partner, by immunizing with a mutant form of the protein that elicits antibodies with greater inhibitory activity than 15 those antibodies elicited by the wild type protein. In one example, mutant proteins are designed using the crystal structure of purified FimCH bound to mannose. Mutant proteins are expressed and used as antigens to elicit antibodies. Thus, this crystal structure, including its coordinates, and methods of designing vaccines and antibodies using information from the crystal structure are included herein. In particular embodiments, this 20 invention relates to mutant bacterial adhesin proteins and active fragments thereof for use in the prevention, diagnosis and treatment of bacterial induced diseases such as those of the urinary tract. The invention encompasses use of mutant proteins as immunogenic agents in vaccine compositions to stimulate an immune response in humans and animals. The invention also encompasses the administration of antibodies to said mutant proteins to 25 humans and animals in an effective amount, to treat, prevent or manage disease or infection. More specifically, the invention relates to the administration of purified mutant adhesin proteins or antibodies directed against said mutant adhesin proteins to a mammalian species as a mechanism to protect the vaccine or antibody recipient against infection by pathogenic bacterial species, including all types of Enterobacteriaceae.

2. BACKGROUND OF THE INVENTION

Urinary tract infections (herein, "UTI") present a disease process that is mediated (or assisted or otherwise induced) by the attachment of bacteria to cells. Escherichia coli is the most common pathogen of the urinary tract, accounting for more than

30

85% of cases of asymptomatic bacteriuria, acute cystitis and acute pyelonephritis, as well as greater than 60% of recurrent cystitis, and at least 35% of recurrent pyelonephritis infections. Furthermore, approximately 25%-30% of women experience a recurrent *E. coli* urinary tract infection within the first 12 months following an initial infection but after a second or third infection the rate of recurrence increases to 60%-75%. Given the high incidence, continued persistence, and significant expense associated with *E. coli* UTI, there is a need for a prophylactic treatment to reduce susceptibility to this disease.

5

10

15

20

25

30

35

Despite the overall prevalence of UTI in women, there have been few efforts to apply novel strategies in order to treat and/or prevent these diseases. Commonly, conventional antibiotics are used to treat these infections, such as treatment with penicillins, cephalosporins, aminoglycosides, sulfonamides and tetracyclines; in the special case of UTI, urinary antiseptics such as nitrofurantoin and nalidixic acid are employed, too. However, emerging antibiotic resistance will in the future hamper the ability to successfully treat UTI. Multiple antibiotic resistance among these uropathogens is increasing.

While many factors contribute to the acquisition and progression of *E. coli* UTI, it is generally accepted that colonization of the urinary epithelium is a required step in the infection process. In a typical course of *E. coli* urinary tract infection, bacteria originate from the bowel, ascend into the bladder, and adhere to the bladder mucosa where they multiply and establish an infection (cystitis) before ascending into the ureters and kidneys. Disruption or prevention of pilus-mediated attachment of *E. coli* to urinary epithelia may prevent or retard the development of UTI. In this regard, a number of studies have pointed to a role for pili in mediating attachment to host uroepithelial cells.

The initiation and persistence of many bacterial infections such as those described above is thought to require the presentation of adhesins on the surface of the microbe in accessible configurations which promote binding events that dictate whether extracellular colonization, internalization or other cellular responses will occur. Adhesins are often components of the long, thin, filamentous, heteropolymeric protein appendages known as pili, fimbriae, or fibrillae (these three terms will be used interchangeably herein). The bacterial attachment event is often the result of a stereo-chemical fit between an adhesin frequently located at the pilus tip and specific receptor architectures on host cells, often comprising carbohydrate structures in membrane associated glycoconjugates.

Uropathogenic strains of *E. coli* express P and type 1 pili that bind to receptors present in uroepithelial cells. The adhesin present at the tip of the P pilus, PapG, binds to the $Gal\alpha(1-4)Gal$ moiety present in the globoseries of glycolipids. Alternatively, the type 1 adhesin, FimH, binds D-mannose present in glycolipids and glycoproteins. Type

1 pili are thought to be important in initiating colonization of the bladder and inducing cystitis, whereas P pili are thought to play a role in ascending infections and the ensuing pyelonephritis.

5

10

15

20

25

30

35

With regard to type 1 pili, tip adhesins and other ancillary subunits also have been identified. FimH is the D-mannose-binding adhesin that promotes attachment of type 1 piliated bacteria to host cells via mannose-containing glycoproteins on eukaryotic cell surfaces. FimC is its periplasmic chaperone protein. It has recently been reported that such chaperones can direct formation of the appropriate native structure of the corresponding adhesin or pilin by inserting a specific fold of the chaperone protein in place of a missing domain or helical strand of the chaperone or pilin. Thus, FimH proteins tend to have their native structure in the presence of such a chaperone but not in its absence (Choudhury et al., 1999, Science 285:1061; Sauer et al., 1999, Science 285:1058). In addition, recent publications have indicated that the required chaperone strand can be inserted into the adhesin or pilin protein, such as FimH, to provide the missing structure and produce the correct native structure.

Sokurenko et al. (1995, J. Bacteriol. 177:3680-86) had found that quantitative variations in mannose-sensitive adhesion of E. coli are due primarily to structural differences in the FimH adhesin. Further research has shown that the ability of the FimH lectins to interact with monomannosyl residues strongly correlates with their ability to mediate E. coli adhesion to uroepithelial cells so that certain phenotypic variants of type 1 fimbriae may contribute more than others to the virulence of E. coli in the urinary tract. (Sokurenko et al., 1997, J. Biol. Chem. 272:17880-6). Heretofore, random point mutations in FimH genes that increase binding of the adhesin to mono-mannose residues (structures abundant in the oligosaccharide moieties of urothelial glycoproteins) had been found to confer increased virulence in the mouse urinary tract (Sokurenko et al., 1998, Proc. Natl. Acad. Sci. USA 95:8922-6).

Antibodies directed against purified whole type 1 or P pili protect against cystitis and pyelonephritis, respectively, in both murine and primate models for these diseases. See Abraham et al., 1985, Infect Immun. 48:625; Roberts et al., 1994, Proc. Natl. Acad. Sci. (USA) 91:11889; and O'Hantey et al., 1985, J. Clin. Invest. 75: 347. However, such protection is limited to either homologous E. coli strains from which the pili used as immunogens were derived, or to a small subset of serologically cross-reactive heterologous strains. Therefore, vaccines composed predominantly of the major structural proteins of pili (i.e., PapA or FimA) appear to be of limited value because antibodies developed against these highly variable proteins are specific for the strains used for immunization.

Vaccination techniques have been developed wherein the vaccine composition is delivered to the subject directly at mucosal tissues, such as gut associated lymphoid tissue, nasopharyngeal lymphoid tissue and bronchial-associated lymphoid tissue, thereby providing localized immunity. Mucosal humoral immunity has been generally thought to come from the secreted form of immunoglobulin, IgA. However, to date, there are no reports of systemic administration of a FimH vaccine composition to a primate which stimulates a humoral immune response sufficient to provide protective immunity at mucosal tissues in humans, with respect to urogenital tract infections. FimH is highly conserved not only among uropathogenic strains of *E. coli*, but also among a wide range of gram-negative bacteria. For example, all Enterobacteriaceae produce FimH. Thus, vaccines incorporating the FimH antigen should exhibit a broad spectrum of protection.

5

10

20

25

30

35

In addition to vaccination, inhibitory antibodies to FimH may be used in a passive immunization approach to elicit protection from infection. This type of approach has been successful used to combat respiratory syncytial virus (RSV) infection. Newborns that were given antibodies directed against RSV intravenously and intramuscularly had decreased incidence of RSV infection. This same group of investigators then examined the ability of hyperimmune serum or purified antibody to protect cotton rats and primates against RSV infection (Prince et al., 1985, Virus Res. 3:193-206; Prince et al., 1990, J. Virol. 64:3091-3092; Hemming et al., 1985, J. Infect. Dis. 152:1083-1087; Prince et al., 1983, Infect. Immun. 42:81-87; and Prince et al., 1985, J. Virol. 55:517-520). Results of these studies suggested that RSV inhibitory antibody given prophylactically inhibited respiratory tract replication of RSV in cotton rats. When given therapeutically, RSV antibody reduced pulmonary viral replication both in cotton rats and in a nonhuman primate model.

While other antigens have been utilized to produce antibodies for diagnosis and for the prophylaxis and/or treatment of bacterial urinary tract infections, there is a need for improved or more efficient vaccines and inhibitory antibodies for use in primates, and more particularly in humans. Such vaccines and inhibitory antibodies should have an improved or enhanced effect in preventing bacterial infections mediated by adhesins and pili sufficient to prevent or treat UTI in humans.

3. BRIEF SUMMARY OF THE INVENTION

Traditional approaches of generating antibody responses to proteins, particularly to inhibit protein function, such as binding to a binding partner, have focused on targeting antibody responses to either a conserved immunogenic linear epitope, a

conformational epitope that mimics native protein structure, or a surface epitope outside of the binding site. The antibody's blocking effect results from agglutination or steric hindrance. The present invention is based, in part, on the inventors' discovery that mutant forms of the bacterial adhesin FimH, which include one or more mutations in a region of FimH critical to mannose binding, induces antibodies with a greater functional inhibitory activity (in this case binding of FimH to mannose or epithelial cells) than those antibodies induced by wild type FimH. Although not intending to be bound by any mechanism of action, the mutant FimH is predicted to adopt a more open conformation in a region critical for mannose binding such that residues that were poorly exposed in the wild type protein can be exploited as epitopes in the mutant protein. Antibodies directed to these once poorly accessible epitopes are highly inhibitory to the adhesin binding to its cellular receptor.

5

10

20

25

30

35

Accordingly, the present invention relates to methods for inducing antibodies having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a protein to its binding partner, by immunization with a mutant form of the protein (i.e., having one or more amino acid modifications relative to the wild type protein or some other reference protein, which may be another mutant protein), whereby the antibodies elicited by the mutant protein have greater functional inhibitory activity than antibodies elicited by the wild-type or reference protein. In particular embodiments, the protein antigen has one or more mutations relative to the wild type or reference protein, which mutations are in regions of the protein involved in protein function (e.g., ligand or receptor binding) and which regions may be poorly exposed to solvent and/or poorly accessible for antibody production in vivo in the wild type protein. The mutations may result in exposing otherwise poorly exposed epitopes that serve as highly potent targets for functional, inhibitory antibodies. In other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations abolish or significantly reduce protein function (for example, but not by way of limitation, binding to a binding partner). In yet other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations result in a protein comprising peptides that bind more tightly to major histocompatibility complex (MHC) molecules resulting in enhanced antigen presentation.

The invention relates to production of high potency inhibitory antibodies against any protein that has a binding partner, for example, against a ligand associated with a receptor-ligand pair, particularly ligands on pathogens involved in binding to host cell receptors. Using pathogen ligands it is possible to develop vaccines that induce antibodies that inhibit binding of the pathogen to host cell receptors, thus preventing infection.

Peptides and proteins that elicit antibodies with greater inhibitory activity and antibodies with greater inhibitory activity are advantageous in that they provide greater protection against infection (or whatever therapeutic or prophylactic effect is desired).

A particular embodiment of the invention provides mutant adhesin proteins and peptides that elicit antibodies that have greater activity in inhibiting binding of the adhesin protein, and/or the pathogen associated therewith, to the corresponding cellular receptor of the adhesin protein; as well as antibodies elicited by immunization with such mutant adhesin proteins and peptides. In one embodiment the adhesin molecule is PapG and the binding partner is a Gala(1-4)Gal.

10

15

20

25

30

35

5

In a preferred embodiment, the invention provides mutant E. coli FimH proteins and peptides that elicit antibodies that more effectively inhibit binding of FimH to mannose than antibodies elicited by wild type FimH (or even other reference mutants of FimH). In particular embodiments, the mutations involve one or more amino acid modifications (e.g., insertions, deletions and, preferably, substitutions) in the canyon region of the FimH molecule, which region is involved in mannose binding. In certain embodiments, the amino acid modifications promote a more open conformation of the FimH protein to expose regions that are poorly exposed in the wild type FimH molecule. In other embodiments, the amino acid modifications significantly reduce or abolish FimHmannose binding. Preferably, the mutations are made in one or more of amino acid residues 1, 13, 46, 47, 48, 52, 54, 62, 67, 75, 133, 135, 137, 138, 140, 142, 154, 156, and 161 of the FimH amino acid sequence depicted in Figure 1 and in SEQ ID NO:4 (or the corresponding residue in a FimH variant or other adhesin molecule as determined by sequence alignment, see e.g., Figure 3). In a preferred embodiment, the amino acid modification (preferably substitution) is at residue 54, 133, or 135 of the amino acid sequence of FimH (Figure 1 and SEQ ID NO:4). In more preferred embodiments, the amino acid residue at position 54 can be substituted with asparagine or alanine; the residue at amino acid position 133 can be substituted with lysine, arginine, glutamate, or histidine; and/or the amino acid residue at position 135 can be substituted with aspartic acid. Such mutant proteins and peptides are particularly useful as vaccines for the prevention of UTI. Further, the invention encompasses molecules having two or more mutations wherein one mutation is of amino acid residue 54, 133, or 135 of the FimH amino acid sequence.

Also encompassed by the invention are vaccine compositions comprising the mutant proteins and polypeptides, and antibodies produced by immunizing with such mutant proteins and polypeptides, as well as methods of vaccination, treatment and prophylaxis using the proteins, polypeptides and antibodies of the invention.

In another embodiment, the antibodies directed against the mutant protein can be administered directly as passive immunization. The present invention is based, in part, on the development of methods for achieving or inducing a prophylactically or therapeutically effective serum titer of an antibody or fragment thereof that immunospecifically binds to a mutant antigen of a pathogen of interest in a mammal by passive immunization with such an antibody or fragment thereof. The present invention also includes the identification of antibodies with higher inhibitory activity which result in increased efficacy for prophylactic or therapeutic uses such that lower serum titers are prophylactically or therapeutically effective, thereby permitting administration of low dosages and/or less frequent administration as compared to other antibody therapeutics.

5

10

15

20

25

30

35

The present invention provides methods of preventing, neutralizing, treating and ameliorating one or more symptoms associated with a pathogen infection in a subject comprising administering to said subject one or more antibodies or fragments thereof which immunospecifically bind to one or more pathogen antigens and display an increased inhibitory activity. Because a lower serum titer of such antibodies or fragment thereof is therapeutically or prophylactically more effective than the effective serum titer of known antibodies, low to moderate doses of said antibodies or antibody fragments can be used to achieve a serum titer effective for the prevention, neutralization, treatment and the amelioration of symptoms associated with a pathogen infection. The use of low doses of antibodies or fragments thereof which immunospecifically bind to one or more pathogen antigens reduces the likelihood of adverse effects. Further, the increased inhibitory activity of the antibodies of the invention or fragments thereof enable less frequent administration of said antibodies or antibody fragments than previously thought to be necessary for the prevention, neutralization, treatment or the amelioration of symptoms associated with a pathogen infection.

The invention further includes co-crystals of a purified FimCH complex bound to a mannose in crystalline form. The invention encompasses the use of the three-dimensional structural representation of this co-crystal to design and/or screen mutant proteins, for example as vaccines, to produce antibodies with these mutant proteins or to design other molecules as therapeutic or prophylactic candidates for drug development. The designing or screening can be conducted using computers and computational programs or actual synthesis and *in vitro* and/or *in vivo* screening. The invention includes the use of the atomic coordinates representing the three-dimensional structure and a machine-readable medium embedded with information that corresponds to a three-dimensional structural representation of the FimCH-mannose complex.

In one aspect, the invention provides crystalline forms of polypeptides corresponding to FimCH bound to a mannose sugar. The FimCH complex of the crystalline form can be a wild type FimCH complex or a mutant FimCH complex. The mutant FimCH complex can comprise a mutant FimC or a mutant FimH or both. For example, the mutant FimCH complex can comprise a truncated mutant of FimC or a truncated mutant of FimH, or both. In certain embodiments of the invention, the mutant FimCH complex can be any mutant FimCH complex described herein. In the co-crystals, the mannose sugar can be any mannose sugar including, for example, mannopentaose, methyl-alpha-D-mannopyranoside, alpha-D-mannopyranoside, mannotriose, an oligomannoside, a dimannoside, etc.

The crystals of the invention include native crystals, in which the crystallized FimCH is substantially pure; heavy-atom derivative crystals, in which the crystallized FimCH is in association with one or more heavy-metal atoms; and co-crystals, in which the crystallized FimCH is in association with one or more compounds, including but not limited to, cofactors, ligands, substrates, substrate analogs, inhibitors, allosteric effectors, etc. to form a crystalline co-complex. Preferably, such compounds bind a catalytic or active site. The co-crystals may be native co-crystals, in which the co-complex is substantially pure, or they may be heavy-atom derivative co-crystals, in which the co-complex is in association with one or more heavy-metal atoms.

In one embodiment, wild-type FimCH alpha-D-mannopyranoside co-crystals of the invention are generally characterized by a unit cell of a=138.077+/-0.2 Å, b=138.130+/-0.2 Å, c=215.352+/-0.2 Å, α =90, β =90.005, γ =90 and are preferably of diffraction quality. In another embodiment of the invention, FimCH Q133N methyl-alpha-D-mannopyranoside co-crystals of the invention crystals of the invention are generally characterized by a unit cell of a=138.349+/-0.2 Å, b=138.334+/-0.2 Å, c=213.212+/-0.2 Å, α =90.000, β =89.983, γ =90.000 and are preferably of diffraction quality. In another embodiment of the invention, truncated FimCH mannopentaose co-crystals of the invention crystals of the invention are generally characterized by a unit cell of a=40.002+/-0.2 Å, b=41.762+/-0.2 Å, c=97.074+/-0.2 Å, α =90, β =90, γ =90 and are preferably of diffraction quality.

30

5

10

15

20

25

In more preferred embodiments, the crystals of the invention are of sufficient quality to permit the determination of the three-dimensional X-ray diffraction structure of the crystalline polypeptide to high resolution, preferably to a resolution of greater than about

3 Å, typically in the range of about 1 Å to about 3 Å, about 1.5 Å to about 3 Å, or about 2 Å to about 3 Å.

The invention also provides methods of making the crystals of the invention. Generally, crystals of the invention are grown by dissolving substantially pure polypeptide in an aqueous buffer that includes a precipitant at a concentration just below that necessary to precipitate the polypeptide. Water is then removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

5

10 -

15

20

25

30

35

Co-crystals of the invention are prepared by soaking a native crystal prepared according to the above method in a liquor comprising the compound of the desired co-complex. Alternatively, the co-crystals may be prepared by co-crystallizing the polypeptide in the presence of the compound according to the method discussed above.

Heavy-atom derivative crystals of the invention may be prepared by soaking native crystals or co-crystals prepared according to the above method in a liquor comprising a salt of a heavy atom or an organometallic compound. Alternatively, heavy-atom derivative crystals may be prepared by crystallizing a polypeptide comprising selenomethionine and/or selenocysteine residues according to the methods described previously for preparing native crystals.

In another aspect, the invention provides machine-computer-readable media embedded with the three-dimensional structural information obtained from the crystals of the invention, or portions or substrates thereof. Such three-dimensional structural information will typically include the atomic structure coordinates of the crystallized polypeptide or co-complex, or the atomic structure coordinates of a portion thereof such as, for example, an active or binding site, but may include other structural information, such as vector representations of the atomic structures coordinates, etc. The types of machine- or computer-readable media into which the structural information is embedded typically include magnetic tape, floppy discs, hard disc storage media, optical discs, CD-ROM, electrical storage media such as RAM or ROM, and hybrids of any of these storage media. Such media further include paper on which is recorded the structural information that can be read by a scanning device and converted into a three-dimensional structure with an OCR. The machine readable media of the invention may further comprise additional information that is useful for representing the three-dimensional structure, including, but not limited to, thermal parameters, chain identifiers, and connectivity information.

The invention is illustrated by way of a working example demonstrating the crystallization and characterization of crystals, the collection of diffraction data, and the determination and analysis of the three-dimensional structure of FimCH.

The atomic structure coordinates and machine readable media of the invention have a variety of uses. For example, the coordinates are useful for solving the three-dimensional X-ray diffraction and/or solution structures of other proteins, including mutant FimCH, co-complexes comprising FimCH, and unrelated proteins, to high resolution. Structural information may also be used in a variety of molecular modeling and computer-based screening applications to, for example, intelligently design mutants of the crystallized FimCH that have altered biological activity and to computationally design and identify compounds that bind the polypeptide or a portion or fragment of the polypeptide, such as the active site.

10

15

25

35

5

3.1 DEFINITIONS

The term "analog" as used herein refers to a polypeptide that possesses a similar or identical function as a particular protein (e.g., a FimH polypeptide or FimCH polypeptide complex), or a fragment thereof, but does not necessarily comprise a similar or identical amino acid sequence or structure of that protein complex or a fragment thereof. A polypeptide that has a similar amino acid sequence refers to a polypeptide that satisfies at least one of the following: (a) a polypeptide having an amino acid sequence that is at least 30%, at least 35%, at least 40%, at least 45%, at least 50%, at least 55%, at least 60%, at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 95% or at least 99% identical to the amino acid sequence of the protein or protein complex or a fragment thereof as described herein; (b) a polypeptide encoded by a nucleotide sequence that hybridizes under stringent conditions to a nucleotide sequence encoding a protein or protein complex of the invention, or fragment thereof, as described herein of at least 20 amino acid residues, at least 25 amino acid residues, at least 40 amino acid residues, at least 50 amino acid residues, at least 60 amino residues, at least 70 amino acid residues, at least 80 amino acid residues, at least 90 amino acid residues, at least 100 amino acid residues, at least 125 amino acid residues, or at least 150 amino acid residues; and (c) a polypeptide encoded by a nucleotide sequence that is at least 30%, at least 35%, at least 40%, at least 45%, at least 50%, at least 55%, at least 60%, at least 65%, at least 70%, at least 75%, at least 80%, at least 85%, at least 90%, at least 95% or at least 99% identical to the nucleotide sequence encoding the protein or protein complex of the invention or a fragment thereof as described herein. A polypeptide with similar structure to a protein or protein complex of the invention or a fragment thereof as described herein refers to a polypeptide that has a similar secondary, tertiary or quaternary structure of said protein or protein complex or a fragment thereof as described herein. The structure of a polypeptide can be determined by methods

known to those skilled in the art, including but not limited to, X-ray crystallography, nuclear magnetic resonance, and crystallographic electron microscopy.

5

10

15

20

25

30:

35

The term "derivative" as used herein refers to a polypeptide that comprises an amino acid sequence of a protein (e.g., FimH) or protein complex (e.g., FimCH) of the invention or a fragment thereof as described herein that has been altered by the introduction of amino acid residue substitutions, deletions or additions. The term "derivative" as used herein also refers to a protein or protein complex of the invention or a fragment thereof that has been modified, i.e., by the covalent attachment of any type of molecule to the polypeptide. For example, but not by way of limitation, a protein or protein complex or a fragment thereof may be modified, e.g., by glycosylation, acetylation, pegylation, phosphorylation, amidation, derivatization by known protecting/blocking groups, proteolytic cleavage, linkage to a cellular ligand or other protein, etc. A derivative of a protein or protein complex or a fragment thereof may be modified by chemical modifications using techniques known to those of skill in the art, including, but not limited to specific chemical cleavage, acetylation, formylation, metabolic synthesis of tunicamycin, etc. Further, a derivative of a protein or protein complex or a fragment thereof may contain one or more non-classical amino acids. A polypeptide derivative possesses a similar or identical function as a protein or protein complex or a fragment thereof described herein.

The term "fragment" as used herein refers to a peptide or polypeptide comprising an amino acid sequence of at least 20 contiguous amino acid residues, at least 25 contiguous amino acid residues, at least 40 contiguous amino acid residues, at least 50 contiguous amino acid residues, at least 60 contiguous amino residues, at least 70 contiguous amino acid residues, at least contiguous 80 amino acid residues, at least contiguous 90 amino acid residues, at least contiguous 100 amino acid residues, at least contiguous 125 amino acid residues, at least 150 contiguous amino acid residues, at least contiguous 200 amino acid residues, or at least contiguous 250 amino acid residues of the amino acid sequence of a protein of the invention, such as FimH.

An "isolated" or "purified" polypeptide or polypeptide complex of the invention or fragment thereof is substantially free of cellular material or other contaminating proteins from the cell or tissue source from which the protein is derived, or substantially free of chemical precursors or other chemicals when chemically synthesized. The language "substantially free of cellular material" includes preparations of a polypeptide or polypeptide complex in which the polypeptide or polypeptide complex is separated from cellular components of the cells from which it is isolated or recombinantly produced. Thus,

a polypeptide or polypeptide complex that is substantially free of cellular material includes preparations of polypeptide or polypeptide complex having less than about 30%, 20%, 10%, or 5% (by dry weight) of heterologous protein (also referred to herein as a "contaminating protein"). When the polypeptide or polypeptide complex is recombinantly produced, it is also preferably substantially free of culture medium, *i.e.*, culture medium represents less than about 20%, 10%, or 5% of the volume of the protein preparation. When the polypeptide or polypeptide complex is produced by chemical synthesis, it is preferably substantially free of chemical precursors or other chemicals, *i.e.*, it is separated from chemical precursors or other chemicals which are involved in the synthesis of the protein. Accordingly such preparations of the polypeptide or polypeptide complex have less than about 30%, 20%, 10%, 5% (by dry weight) of chemical precursors or compounds other than the polypeptide or polypeptide complex of interest. In a preferred embodiment, polypeptides or polypeptide complexes or fragments thereof of the invention are isolated or purified.

5

10

15

20

25

30

35

An "isolated" nucleic acid molecule is one which is separated from other nucleic acid molecules which are present in the natural source of the nucleic acid molecule but excludes when the nucleic acid is present as part of a cDNA library. Moreover, an "isolated" nucleic acid molecule, such as a cDNA molecule, can be substantially free of other cellular material, or culture medium when produced by recombinant techniques, or substantially free of chemical precursors or other chemicals when chemically synthesized.

"Plasmids" are designated by a lower case p preceded and/or followed by capital letters and/or numbers. The starting plasmids herein are either commercially available, publicly available on an unrestricted basis, or can be constructed from available plasmids in accord with published procedures. In addition, equivalent plasmids to those described are known in the art and will be apparent to the ordinarily skilled artisan.

The term "attachment domain" refers to the portion of a polypeptide that mediates binding between the polypeptide and a second moiety. The second moiety can comprise cell surface polypeptides and/or polysaccharides. The attachment domain for a FimH polypeptide, which is a type 1 adhesin protein produced by *E. coli*, is depicted in Figure 2E.

The term "canyon region" refers to the region of the FimH polypeptide (or related adhesin) whose surface comprises residues 1, 13, 46, 47, 48, 52, 54, 133, 135, 137, 138, 140, and 142 of FimH (Figure 2) as surface residues of the canyon structure or corresponding residues of a FimH variant or other adhesin as determined by sequence alignment and/or structural comparison.

The term "associated ligand" as used herein refers to a ligand that has an inherent function associated with the recited protein (e.g., binding, such as receptor-ligand binding) and, preferably, does not include an antigen-antibody relationship. As an example, an associated ligand to PapG is a $Gal\alpha(1-4)Gal$ moiety. As another example, an associated ligand to FimH is a mannose moiety.

5

10

15

20

25

30

35

The term "periplasmic chaperone" is defined as a protein localized in the periplasm of bacteria that is capable of forming complexes with a variety of chaperone-binding proteins via recognition of a common binding epitope (or epitopes). Chaperones perform several functions. They serve as templates upon which proteins exported from the bacterial cell into the periplasm fold into their native conformations. Association of the chaperone-binding protein with the chaperone also serves to protect the binding proteins from degradation by proteases localized within the periplasm, increases their solubility in aqueous solution, and leads to their sequentially correct incorporation into an assembling pilus. Chaperone proteins are a class of proteins in gram-negative bacteria that are involved in the assembly of pili by mediating such assembly, but are not incorporated into the structure. PapD is the periplasmic chaperone protein mediating the assembly of pili for P piliated bacteria and FimC is the periplasmic chaperone protein that mediates assembly of type 1 pili in bacteria.

The term "fusion protein" as used herein refers to a polypeptide that comprises an amino acid sequence of a polypeptide or fragment thereof and an amino acid sequence of a heterologous polypeptide (e.g., FimH conjugated to FimC).

The term "FimH antigen" refers to a FimH polypeptide or fragment thereof to which an antibody or antibody fragment immunospecifically binds. A FimH antigen also refers to an analog or derivative of a FimH polypeptide or fragment thereof to which an antibody or antibody fragment immunospecifically binds.

The term "FimCH complex" refers to a complex containing both a FimH and a FimC polypeptide preferably in a 1:1 ratio in the complex.

The terms "pili," "fimbriae," and "fibrillae" are used herein to refer to heteropolymeric protein structures located on the extracellular surface of bacteria, most commonly gram-negative bacteria. Typically these structures are anchored in the outer membrane. Throughout this specification the terms pilus, pili, fimbriae, and fibrilla will be used interchangeably.

The term "substantially similar structure" as used herein refers to a mutant FimH that, although in a more open conformation, retains the general conformation of the wild type protein.

The term "antibodies or fragments that immunospecifically bind to a FimH antigen" as used herein refers to antibodies or fragments thereof that specifically bind to a FimH polypeptide or a fragment of a FimH polypeptide and do not non-specifically bind to other polypeptides. Antibodies or fragments that immunospecifically bind to a FimH polypeptide or fragment thereof may have cross-reactivity with other antigens. Preferably, antibodies or fragments that immunospecifically bind to a FimH polypeptide or fragment thereof do not cross-react with other antigens. Antibodies or fragments that immunospecifically bind to a FimH polypeptide can be identified, for example, by immunoassays or other techniques known to those of skill in the art.

5

10

15

20

25

30

35

The term "Fab fragment" as used herein refers to a fragment of an antibody corresponding to an intact light chain associated with a V_H-C_γ1 fragment of the heavy chain. Although these fragments retain the ability to bind antigen, they are no longer bivalent and thus have lost the ability to aggregate antigen. Fab fragments may be generated by any technique known to those of skill in the art. For example, Fab fragments of the invention may be produced by proteolytic cleavage of immunoglobulin molecules, using enzymes such as papain. Techniques to recombinantly produce Fab fragments can also be employed using methods known in the art such as those disclosed in PCT publication WO 92/22324; Mullinax et al., 1992, BioTechniques 12:864-869; and Sawai et al., 1995, AJRI 34:26-34; and Better et al., 1988, Science 240:1041-1043 (said references incorporated herein by reference in their entireties).

The term "functional inhibitory activity" (in some cases "inhibitory activity") means the ability of an antibody to inhibit or reduce the binding of a protein for a binding partner. For example, the functional, inhibitory activity of an anti-FimH antibody is the ability of the antibody to inhibit or reduce the binding of FimH to a mannose moiety (e.g., mono- or tri-mannose).

The term "passive immunization" as used herein refers to the administration of immune serum or purified antibodies or fragments thereof directly to a patient. Immune serum or purified antibodies can be given prophylactically to inhibit infection or therapeutically to reduce or eliminate infection. This is distinguished from immunization of a patient with a protein to direct an *in vivo* immune response to produce antibodies.

To determine the percent identity of two amino acid sequences or of two nucleic acid sequences, the sequences are aligned for optimal comparison purposes (e.g., gaps can be introduced in the sequence of a first amino acid or nucleic acid sequence for optimal alignment with a second amino acid or nucleic acid sequence). The amino acid residues or nucleotides at corresponding amino acid positions or nucleotide positions are

then compared. When a position in the first sequence is occupied by the same amino acid residue or nucleotide as the corresponding position in the second sequence, then the molecules are identical at that position. The percent identity between the two sequences is a function of the number of identical positions shared by the sequences (i.e., % identity = number of identical overlapping positions/total number of positions x 100%). In one embodiment, the two sequences are the same length.

5

10

15

20

25

30

35

4 can be used.

The determination of percent identity between two sequences can also be accomplished using a mathematical algorithm. A preferred, non-limiting example of a mathematical algorithm utilized for the comparison of two sequences is the algorithm of Karlin and Altschul, 1990, Proc. Natl. Acad. Sci. U.S.A. 87:2264-2268, modified as in Karlin and Altschul, 1993, Proc. Natl. Acad. Sci. U.S.A. 90:5873-5877. Such an algorithm is incorporated into the NBLAST and XBLAST programs of Altschul et al., 1990, J. Mol. Biol. 215:403. BLAST nucleotide searches can be performed with the NBLAST nucleotide program parameters set, e.g., for score=100, wordlength=12 to obtain nucleotide sequences homologous to a nucleic acid molecules of the present invention. BLAST protein searches can be performed with the XBLAST program parameters set, e.g., to score-50, wordlength=3 to obtain amino acid sequences homologous to a protein molecule of the present invention. To obtain gapped alignments for comparison purposes, Gapped BLAST can be utilized as described in Altschul et al., 1997, Nucleic Acids Res. 25:3389-3402. Alternatively, PSI-BLAST can be used to perform an iterated search which detects distant relationships between molecules (Id.), When utilizing BLAST, Gapped BLAST, and PSI-Blast programs, the default parameters of the respective programs (e.g., of XBLAST and NBLAST) can be used (e.g., http://www.ncbi.nlm.nih.gov). Another preferred, non-limiting example of a mathematical algorithm utilized for the comparison of sequences is the algorithm of Myers and Miller, 1988, CABIOS 4:11-17. Such an algorithm is incorporated in the ALIGN program (version 2.0) which is part of the GCG sequence alignment software package. When utilizing the ALIGN program for comparing amino acid sequences, a PAM120 weight residue table, a gap length penalty of 12, and a gap penalty of

The percent identity between two sequences can be determined using techniques similar to those described above, with or without allowing gaps. In calculating percent identity, typically only exact matches are counted.

The term "selenomethionine mutant" as used herein refers to a mutant which includes at least one selenomethionine (SeMet) residue, typically by substitution of a Met residue of the wild-type sequence with a SeMet residue, or by addition of one or more

SeMet residues at one or both termini. Preferred SeMet mutants are those in which each Met residue is substituted with a SeMet residue.

The term "cysteine mutant" as used herein refers to a mutant in which at least one cysteine residue of the wild-type sequence is replaced with another residue, preferably with a Ser (S) residue. The term can also refer to a mutant in which a non-cysteine residue, preferably a Ser (S) residue, of the wild-type sequence is replaced with a cysteine residue.

5

10

15

20

25

35

The term "selenocysteine mutant" as used herein refers to a mutant which includes at least one selenocysteine (SeCys) residue, typically by substitution of a Cys residue of the wild-type sequence with a SeCys residue, or by addition of one or more SeCys residues at one or both termini. The term can also refer to a cysteine mutant in which at least one Cys residue is substituted with a SeCys residue. Preferred SeCys mutants are those in which each Cys residue is substituted with a SeCys residue.

The term "crystal" as used herein refers to a composition comprising a polypeptide in crystalline form. The term "crystal" includes native crystals, heavy-atom derivative crystals and co-crystals, as defined herein.

The term "native Crystal" as used herein refers to a crystal wherein the polypeptide is substantially pure. As used herein, native crystals do not include crystals of polypeptides comprising amino acids that are modified with heavy atoms, such as crystals of selenomethionine mutants, selenocysteine mutants, etc.

The term "heavy-atom derivative crystal" as used herein refers to a crystal wherein the polypeptide is in association with one or more heavy-metal atoms. As used herein, heavy-atom derivative crystals include native crystals into which a heavy metal atom is soaked, as well as crystals of selenomethionine mutants and selenocysteine mutants.

The term "co-crystal" as used herein refers to a composition comprising a co-complex, as defined above, in crystalline form. Co-crystals include native co-crystals and heavy-atom derivative co-crystals.

The term "diffraction quality crystal" as used herein refers to a crystal that is well-ordered and of a sufficient size, i.e., at least 10µm, preferably at least 50µm, and most preferably at least 100µm in its smallest dimension such that it produces measurable diffraction to at least 3 Å resolution, preferably to at least 2 Å resolution, and most preferably to at least 1.5 Å resolution or lower. Diffraction quality crystals include native crystals, heavy-atom derivative crystals, and co-crystals.

The term "unit cell" as used herein refers to the smallest and simplest volume element (i.e., parallelpiped-shaped block) of a crystal that is completely representative of the unit or pattern of the crystal, such that the entire crystal can be generated by translation of

the unit cell. The dimensions of the unit cell are defined by six numbers: dimensions a, b and c and angles α , β and γ (Blundel *et al.*, 1976, Protein Crystallography, Academic Press.). A crystal is an efficiently packed array of many unit cells.

The term "triclinic unit cell" as used herein refers to a unit cell in which $a\neq b\neq c$ and $\alpha\neq \beta\neq \gamma$.

5

10

20

25

30

35

The term "monoclinic unit cell" as used herein refers to a unit cell in which $a\neq b\neq c$; $\alpha=\gamma=90^{\circ}$; and $\beta\neq 90^{\circ}$, defined to be $\geq 90^{\circ}$.

The term "orthorhombic unit cell" as used herein refers to a unit cell in which $a \neq b \neq c$; and $\alpha = \beta = \gamma = 90^{\circ}$.

The term "tetragonal unit cell" as used herein refers to a unit cell in which $a=b\neq c$; and $\alpha=\beta=\gamma=90^{\circ}$.

The term "trigonal/rhombohedral unit cell" as used herein refers to a unit cell in which a=b=c; and α = β = γ +90°.

The term "trigonal/hexagonal unit cell" as used herein refers to a unit cell in which a=b=c; $\alpha=\beta=90^{\circ}$; and $\gamma=120^{\circ}$.

The term "cubic unit cell" as used herein refers to a unit cell in which a=b=c; and $\alpha=\beta=\gamma=90^{\circ}$.

The term "crystal lattice" as used herein refers to the array of points defined by the vertices of packed unit cells.

The term "space group" as used herein refers to the set of symmetry operations of a unit cell. In a space group designation (e.g., C2) the capital letter indicates the lattice type and the other symbols represent symmetry operations that can be carried out on the unit cell without changing its appearance.

The term "asymmetric unit" as used herein refers to the largest aggregate of molecules in the unit cell that possesses no symmetry elements that are part of the space group symmetry, but that can be juxtaposed on other identical entities by symmetry operations.

The term "crystallographically-related dimer" as used herein refers to a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer coincide with the symmetry axes or planes of the crystal lattice.

The term "non-crystallographically-related dimer" as used herein refers to a dimer of two molecules wherein the symmetry axes or planes that relate the two molecules comprising the dimer do not coincide with the symmetry axes or planes of the crystal lattice.

The term "isomorphous replacement" as used herein refers to the method of using heavy-atom derivative crystals to obtain the phase information necessary to elucidate

the three-dimensional structure of a crystallized polypeptide (Blundel et al., 1976, Protein Crystallography, Academic Press.).

5

10

15

20

25

30

35

The terms "multi-wavelength anomalous dispersion" or "MAD" as used herein refers to a crystallographic technique in which X-ray diffraction data are collected at several different wavelengths from a single heavy-atom derivative crystal, wherein the heavy atom has absorption edges near the energy of incoming X-ray radiation. The resonance between X-rays and electron orbitals leads to differences in X-ray scattering from absorption of the X-rays (known as anomalous scattering) and permits the locations of the heavy atoms to be identified, which in turn provides phase information for a crystal of a polypeptide. A detailed discussion of MAD analysis can be found in Hendrickson, 1985, *Trans. Am. Crystallogr. Assoc.*, 21:11; Hendrickson *et al.*, 1990, *EMBO J.* 9:1665; and Hendrickson, 1991, *Science* 4:91.

The terms "single wavelength anomalous dispersion" or "SAD" as used herein refers to a crystallographic technique in which X-ray diffraction data are collected at a single wavelength from a single native or heavy-atom derivative crystal, and phase information is extracted using anomalous scattering information from atoms such as sulfur or chlorine in the native crystal or from the heavy atoms in the heavy-atom derivative crystal. The wavelength of X-rays used to collect data for this phasing technique need not be close to the absorption edge of the anomalous scatterer. A detailed discussion of SAD analysis can be found in Brodersen et al., 2000, *Acta Cryst.*, D56:431-441.

The terms "single isomorphous replacement with anomalous scattering" or "SIRAS" as used herein refers to a crystallographic technique that combines isomorphous replacement and anomalous scattering techniques to provide phase information for a crystal of a polypeptide. X-ray diffraction data are collected at a single wavelength, usually from a single heavy-atom derivative crystal. Phase information obtained only from the location of the heavy atoms in a single heavy-atom derivative crystal leads to an ambiguity in the phase angle, which is resolved using anomalous scattering from the heavy atoms. Phase information is therefore extracted from both the location of the heavy atoms and from anomalous scattering of the heavy atoms. A detailed discussion of SIRAS analysis can be found in North, 1965, *Acta Cryst.* 18:212-216; Matthews, 1966, *Acta Cryst.* 20:82-86.

The term "molecular replacement" as used herein refers to the method of calculating initial phases for a new crystal of a polypeptide whose structure coordinates are unknown by orienting and positioning a polypeptide whose structure coordinates are known within the unit cell of the new crystal so as to best account for the observed diffraction pattern of the new crystal. Phases are then calculated from the oriented and positioned

polypeptide and combined with observed amplitudes to provide an approximate Fourier synthesis of the structure of the polypeptides comprising the new crystal. (Lattman, 1985, *Methods in Enzymology* 115:55-77; Rossmann, 1972, "The Molecular Replacement Method," Int. Sci. Rev. Ser. No. 13, Gordon & Breach, New York.).

The term "having substantially the same three-dimensional structure" as used herein refers to a polypeptide that is characterized by a set of atomic structure coordinates that have a root mean square deviation (r.m.s.d.) of less than or equal to about 2 Å, or less than or equal to about 1 Å, when superimposed onto the atomic structure coordinates of Table 14 when at least about 50% to 100% of the $C\alpha$ atoms of the coordinates are included in the superposition.

The term " $C\alpha$ " as used herein refers to the alpha carbon of an amino acid residue.

4. BRIEF DESCRIPTION OF THE DRAWINGS

Figures 1 A-D: Wild type FimC and FimH nucleic and amino acid sequence. (A) nucleic acid sequence of FimC (SEQ ID NO:1); (B) amino acid sequence of FimC (SEQ ID NO:2); (C) nucleic acid sequence of FimH (SEQ ID NO:3); (D) amino acid sequence of FimH (SEQ ID NO:4) (from Choudhury et al. 1999, *Science* 285:1061 incorporated herein by reference).

20

25

30

5

10

Figures 2 A-E: Crystal structure of FimCH chaperone-adhesin complex bound to α -D-mannose. (A) Overall structure of FimCH with the two domains of the chaperone FimC (black) and the pilin domain of FimH (gray). As demonstrated previously, the receptor-binding domain of FimH is an elongated eleven-stranded β -barrel comprised of residues Phe1 to Thr158, and is connected via a flexible linker to the pilin domain of FimH. (B) The bound mannose receptor is shown at a 90° rotation of the receptor binding domain shown in (A). The mannose, the mannose-interacting residues, and the residues of the hydrophobic ridge around the pocket are shown in ball-and stick model. (C) Stereo presentation of omit electron density at 4 σ (F_o-F_c) for the α -D-mannoside bound in pocket of FimH. The interacting amino acids are shown in ball-and-stick with hydrogen bonds shown by dotted lines. (D) The receptor binding domain of FimH displaying the electrostatic potential surface, with positively and negatively charged residues shaded and hydrophobic residues labeled. (E) The tip of the FimH receptor binding domain is shown.

35

Figure 3: Alignment of deduced amino acid sequences of the FimH lectin-binding

domain from representative clinical isolates. The regions involved in mannose binding are shown highlighted in gray. The other positions shown were found to be heterogenous among throughout all the FimH sequences examined. The sequences that are not shown were found to be conserved also among all isolates. UTI strain J96 was used as the consensus sequence. Amino acid residues that are identical to that of J96 were indicated by "." while the residues different from the consensus were indicated.

Figure 4: FimH mutants were complexed with FimC, another type 1 pilus protein. Wild type FimC was found to associate with wild type FimH, the vaccine composition of wild type FimH, FimH N46A, FimH N46D, FimH Q133K, and FimH D140E equally well as assayed by ELISA using an anti-FimC antibody. closed circles=FimH N46A; open circles=FimH D140E; closed triangles=FimH Q133K; open triangles=FimH N46D; closed squares=vaccine composition of wild type FimH; open squares=wild type FimH.

Figures 5 A-B: Binding of purified FimCH complexes to mono-mannose coated beads and their elution by methyl-α-D-mannopyranosides. (A) A Coomassie-stained SDS-PAGE gel shows that most FimH mutants still retained the ability to bind mono-mannose coated beads ("bound"). (A) A Coomassie-stained SDS-PAGE gel shows that bound mutant FimH proteins were eluted-off with methyl-α-D-mannopyranosides ("eluted"). (B)

The ratio of bound to eluted FimH protein. Asterisk indicates no FimH was bound to the bead initially.

Figures 6 A-B: Binding of purified FimCH complexes to mannose as assayed by ELISA. Comparison of different mutant FimCH proteins in their ability to bind (A) monomannose and (B) tri-mannose. In upper panels, closed square with unbroken line=WT control, closed diamond with dotted line=N46D, closed circle=D54A, closed triangle=D54N, closed square with dashed line=S62A, opened circle=Q133K, closed upside down triangle=Q133N, closed diamond with dashed line=Q133A, half filled diamond=N135D, bottom filled square=N135A, top filled square=D140N, star=D140A, and open triangle=D140E. In lower panels, closed circle and open square=WT control, open circle=I13A, closed upside down triangle=Y48A, open upside down triangle=I52A, closed square=Q133E, closed diamond=Q133H, open diamond=Q133R, filled triangle=N135D, open triangle=Y137A.

25

30

5

10

Figures 7 A-I: Mutant FimH expressing E. coli binding to mannose. Comparison of different mutant FimCH proteins in their ability to bind (A) monomnnose and (B) trimannose. Comparison of monomnnose and trimannose binding of PmmB66 expressing wild type FimCH with (C) untransfected PmmB66; (D) PmmB66 expressing FimCH N46A; (E) PmmB66 expressing FimCH N46D; (F) PmmB66 expressing FimCH D140E; (G) PmmB66 expressing FimCH Q133K; and (H) PmmB66 expressing FimCH S62A. (I) Mutant FimH expressing E. coli binding to control plates coated with the polyclonal anti-E. coli antibody. In panels A, B, and I, closed circle=PmmB66FimH, open circle=WT FimH, filled triangle=N46A, open triangle=N46D, closed square=D140E, open square=Q133K, 10 diamond=S62A. In panels C-H, closed triangle=WT FimH binding to mono-mannose, open triangle=WT FimH binding to tri-mannose, closed circle=FimH binding to mono-mannose, open circle=FimH binding to tri-mannose.

5

25

Figures 8 A-B: Binding and invasion of 5637 cells. (A) AAEC185/pUT2002 15 bacteria complemented with different FimH variants did not exhibit any significant binding to 5637 cells with the exception of FimCH S62A and FimCH N46D mutants. Results were obtained from at least two different infection experiments with duplicate wells in each experiment. X-axis represents the percent cell association of total input bacteria, which includes both the surface bound and invaded bacteria. (B) Bound bacteria expressing mutant 20 FimH proteins showed a similar degree of invasion into 5637 cells. Results shown are from one representative experiment.

Figures 9 A-K: Binding of type 1 piliated-bacteria to human bladder sections. AAEC185/pUT2002 bacteria complemented with (A) WT; (C) S62A; (E) N46A; (F) N46D; (H) D54A; (I) Q133A; and (J) Q133K, FimH expression and (K) vector control plasmids were used in the binding assay. Binding of (B) WT; (D) S62A; and (G) N46D can be inhibited by methyl-α-D-mannopyranosides.

Figures 10 A-C: Results from an ELISA of levels of anti-FimH specific IgG 30 polyclonal antibodies in serum of vaccinated mice. Titers are shown as endpoint dilutions which are measured by an ELISA where FimH T3 (a histidine-tagged fusion protein composed of the first 165 amino acids of FimH) is the capture antigen and the detection antibody is specific to IgG. A booster immunization was given 3 weeks after the initial immunization. Doses of protein at each injection were either 4.0, 1.6, 0.64, and 0.26 µg (as 35 indicated). Wild type FimCH was used as an immunogen for vaccination and resulting

antibody titers were compared to those seen for mutant protein: (A) FimCH N46D; (B) FimCH D140E; and (C) FimCH Q133K. WT FimCH is depicted by open symbols while indicated mutant FimCH is depicted by closed symbols. square=4ug, circle=1.6ug, triangle=0.64 ug, diamond=.026 ug. star=MF 59 adjuvant alone.

5

10

15

20

25

30

35

Figures 11 A-C: Hemagglutination assay inhibition by polyclonal antibodies. *E. coli* was preincubated with increasing dilutions of a polyclonal antibody raised against the indicated FimCH complex. The FimCH complex on the bacteria was tested for its ability to bind the mannose present on the erythrocytes in the presence of the polyclonal antibody. Decreased mean channel fluorescence in the presence of the antibody indicated that the polyclonal antibody inhibited FimCH binding in this assay. Preincubation with polyclonal antibodies raised against (A) FimCH Q133 E, FimCH Q133H, and WT FimCH and (C) FimCH N135D, FimCH Q133R, and WT FimCH inhibited bacteria binding to the erythrocytes very strongly. (B and D) Control antiserum from animals that were either not immunized or immunized with MF59 adjuvant alone showed no inhibition.

Figures 12 A-E: Polyclonal antibody inhibition of *E. coli* NU14 binding to J82 human bladder cells as measured by multiple channel fluorescence (MCF) in log2 scale. Polyclonal antibodies raised against the indicated mutant or wild type FimCH protein were preincubated with bacteria cells before addition to bladder cells for binding: (A) anti-FimCH N46D (8 week sera used after a boost at week 4); (B) anti-FimCH D140E (8 week sera used after a boost at week 4); and (C) anti-FimCH Q133K (8 week sera used after a boost at week 4). For wild type FimCH and FimCH Q133K, an additional boost at week 18 was given. Inhibitory assays were done with antisera from week 16 (darker bar) and week 20 (lighter bar): (D) anti-FimCH; and (E) anti-FimCH Q133K.

Figure 13: Passive immunization with polyclonal antibodies generated with mutant FimCH protein. Mice were administered 1 mg of polyclonal antibody 4 hours prior to a large bolus challenge with *E. coli* Nu14. After 48 hours, mice were sacrificed to harvest the bladders. The number of CFUs were determined. A decrease in the number of CFUs indicates that the passive immunization had a protective ability.

Figure 14: Hemagglutination assay inhibition by monoclonal antibody (MAB). *E. coli* was preincubated with increasing dilutions of the indicated MAB clone. The FimCH complex on the bacteria was tested for its ability to bind the mannose present on the

erythrocytes in the presence of the MAB. Decreased mean channel fluorescence indicated that the MAB clone was inhibitory in this assay. Preincubation with clone 1A7 inhibited bacteria binding to the erythrocytes very strongly. Clones 1C10 and 3E11 also inhibited bacteria binding when the MABs were supplied in larger quantities. Clones 1F2, 2B2, and 1C8 did not show an inhibitory activity.

5

10

25

30

35

Figure 15: Hemagglutination assay inhibition by MAB clone 1A7. *E. coli* was preincubated with increasing dilutions of MAB clone 1A7. The FimCH complex on the bacteria was tested for its ability to bind the mannose present on the erythrocytes in the presence of the MAB. Decreased mean channel fluorescence indicated that the MAB clone was inhibitory in this assay. (A) Preincubation with clone 1A7 inhibited bacteria binding to the erythrocytes very strongly. (B) Controls showed that this inhibitory activity was due to preincubation with MAB clone 1A7.

Figure 16: Tri-mannose binding inhibition by MAB. An ELISA assay was used to measure the ability of the FimCH complex on bacteria to bind tri-mannose in the presence of the MAB. A decrease in OD₄₅₀ indicated that bacteria were inhibited from binding to the tri-mannose. Both MAB clone 1A7 and 1C10 inhibited binding while MAB clone 1C8 did not. closed circle=1A7, open circle=1C8, upside down triangle=1C10, triangle=anti B19 negative control.

Figure 17: Hemagglutination assay inhibition by Fab fragments. *E. coli* was preincubated with increasing dilutions of the indicated Fab fragment. The FimCH complex was tested for its ability to bind the mannose present on the erythrocytes in the presence of the Fab fragment. Decreased mean channel fluorescence indicates that the Fab fragment was inhibitory in this assay.

Figure 18: Passive immunization with MABs generated with mutant FimCH protein. Mice were administered 1 mg of MAB 4 hours prior to a large bolus challenge with *E. coli* Nu14. After 48 hours, mice were sacrificed to harvest the bladders. The number of CFUs were determined. A decrease in the number of CFUs indicates that the passive immunization had a protective ability.

Figures 19 A-B: Ball-and-stick presentation of changes in the structure of the mannose binding pocket between (A) wild type FimCH and (B) Q133N FimCH: Hydrogen

bonds are shown as dotted lines and aromatic contacts are shown as dashed lines. Water molecules are labeled as W1 and/or W2.

5

10

15

20

25

30

35

5. <u>DETAILED DESCRIPTION OF THE INVENTION</u>

The present invention is based, in part, on the inventors' discovery that certain mutant forms of the bacterial adhesin FimH, which have one or more mutations in a canyon region of FimH critical to mannose binding, induced antibodies with a greater functional inhibitory activity (in this case inhibiting binding of FimH to mannose or epithelial cells) than those antibodies induced by wild type FimH. Although not intending to be bound by any mechanism of action, the mutant FimH is predicted to adopt a more open conformation in a region critical for mannose binding such that residues that were poorly exposed in the wild type protein can be exploited as epitopes in the mutant protein. Antibodies directed to these once inaccessible epitopes are highly inhibitory to the adhesin.

Accordingly, the present invention relates to methods for inducing antibodies having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a protein to its binding partner, by immunization with a mutant form of the protein (i.e., having one or more amino acid modifications relative to the wild type protein or some other related reference protein, which may be another mutant protein), whereby the antibodies elicited by the mutant protein have greater functional inhibitory activity than antibodies elicited by the wild-type or reference protein. In particular embodiments, the protein antigen has one or more mutations relative to the wild type or reference protein, which mutations are in regions of the protein involved in protein function (e.g., ligand or receptor binding) and which regions may be poorly exposed to solvent and/or poorly accessible for antibody production in vivo in the wild type protein. The mutations may result in exposing otherwise buried epitopes that serve as highly potent targets for functional, inhibitory antibodies. In other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations abolish or significantly reduce protein function (for example, but not by way of limitation, binding to a binding partner). In yet other embodiments, the protein antigen has one or more mutations relative to the wild type protein or reference protein, which mutations result in a protein comprising peptides that bind more tightly to MHC molecules resulting in enhanced antigen presentation.

The invention relates to production of high potency inhibitory antibodies against any protein that has a binding partner, for example, against a ligand associated with a receptor-ligand pair, particularly ligands on pathogens involved in binding to host cell receptors. Using pathogen ligands is it possible to develop vaccines that induce antibodies

that inhibit binding of the pathogen to host cell receptors, thus preventing infection. Additionally, the antibodies directed against the pathogen protein can be administered directly as passive immunization. Peptides and proteins that elicit antibodies with greater inhibitory activity and antibodies with greater inhibitory activity are advantageous in that they provide greater protection against infection (or whatever therapeutic or prophylactic effect is desired).

5

10

25

30

35

Each of the above-described peptides and proteins can be designed or generated using information from the complex of FimCH-mannose in crystalline form, such information includes but is not limited to the three-dimensional structure. Thereafter, antibodies to the novel mutant peptides or proteins can be generated.

5.1 MUTANT PROTEINS AS ANTIGENS FOR HIGH POTENCY INHIBITORY ANTIBODIES

The present invention relates to methods for inducing antibodies having
enhanced functional inhibitory activity, particularly enhanced ability to block binding of a
protein to its binding partner, by immunization with a mutant form of the protein (i.e.,
having one or more amino acid modifications relative to the wild type protein or some other
related reference protein, which may be another mutant protein), whereby the antibodies
elicited by the mutant protein have greater functional inhibitory activity than antibodies
elicited by the wild-type or reference protein.

In particular embodiments, the protein antigen has one or more mutations relative to the wild type or reference protein, which mutations are in regions of the protein involved in protein function (e.g., ligand or receptor binding) and which regions are poorly exposed to solvent and/or poorly accessible for antibody production in vivo in the wild type protein. The mutations may result in exposing otherwise poorly exposed epitopes that serve as highly potent targets for functional, inhibitory antibodies. Such residues can be identified by any means known in the art, preferably, by computer modeling, to identify residues critical for a particular protein conformation, which residues, when modified (preferably, substituted with another amino acid residue), result in a more open protein conformation. In preferred embodiments, the more open protein conformation exposes one or more regions of the protein that are poorly exposed in the wild type or reference protein, more preferably, these one or more regions are involved (in some aspects, critical for) protein binding to a binding pair. Preferably, the amino acid residue that is substituted differs in hydrophobicity, polarity, size, or charge from the amino acid present at that position in the wild type or reference protein. Additionally, libraries of random mutants can be generated at one or more

residues identified by modeling or other methods to be critical for protein conformation, particularly in regions important in protein binding to a binding partner (e.g., ligand binding to an associated receptor), and/or the mutation of which is predicted to expose otherwise poorly exposed regions, preferably those involved in protein binding. Such libraries of randomly mutated proteins can be screened using methods well known in the art for mutant proteins that elicit antibodies that have higher functional inhibitory activity than the antibodies elicited by a wild type or reference protein.

5

10

15

20

25

30

35

In other embodiments, the protein antigen has one or more mutations (i.e., amino acid modifications) relative to the wild type protein, which mutations abolish or significantly reduce protein function (for example, but not by way of limitation, binding to a binding partner). The residues to be mutated can be identified by any method known in the art for identifying residues critical for ligand binding, for example, but not by way of limitation, protein modeling and mutational analysis. Preferably, the amino acid residue that is substituted differs in hydrophobicity, polarity, size, or charge from the amino acid present at that position in the wild type or reference protein. Additionally, libraries of random mutants can be generated at one or more residues identified by modeling or other methods to be critical for ligand binding. Such libraries of randomly mutated protein can be screened for mutant proteins that have reduced or no binding activity and/or the ability to elicit antibodies that have higher functional inhibitory activity than the antibodies elicited by a wild type or reference protein.

In yet other embodiments, the protein antigen has one or more mutations relative to the wild type protein, which mutations result in a protein comprising peptides that bind more tightly to MHC molecules resulting in enhanced antigen presentation.

The mutant proteins of the invention may have any number of mutations relative to the corresponding wild type protein or reference protein as long as they elicit antibodies that have greater functional inhibitory activity than antibodies elicited by the wild type or reference protein. In certain embodiments, the protein contains 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 15, 20 or more than 25 mutations. In certain embodiments, the protein also contains mutations relative to the wild type or reference protein that do not affect (or even decrease) the ability of the protein to elicit antibodies with a greater functional inhibitory activity than those elicited by the wild type or reference protein, as long as the mutant protein is able to elicit such high potency inhibitory antibodies. The invention also includes fragments of the mutant proteins that elicit antibodies with greater inhibitory activity than the wild type or reference protein and/or than the corresponding fragment of the wild type or reference protein.

The invention relates to producing mutants of any protein that is a member of a binding pair, including proteins that bind non-protein molecules, such as carbohydrates including lectins, lipids, steroids, non-peptide hormones, or other small molecules. In particular, such proteins are members of a ligand-receptor pair. Either the ligand or the receptor may be the antigen that is mutated. Such mutated ligand or receptor can then be used to raise antibodies with enhanced activity to block ligand-receptor binding. In a preferred embodiment, the binding pair is not an antigen-antibody binding pair.

5

10

15

20

25

30

35

In preferred embodiments, the invention relates to methods for inducing antibodies having enhanced functional inhibitory activity, particularly enhanced ability to block binding of a pathogenic protein to its host cell receptor, by immunization with a mutant form of the pathogenic protein (*i.e.*, having one or more amino acid modifications relative to the wild type or reference protein), whereby the antibodies elicited by the mutant pathogenic protein have greater functional inhibitory activity than antibodies elicited by the wild-type protein. In particular embodiments, the pathogenic protein antigen has one or more mutations relative to the wild type or reference pathogenic protein, which mutations result in exposing regions of the protein which are poorly exposed to solvent and/or not accessible for antibody production *in vivo* in the wild type protein. By way of example but not limitation, the mutations may result in exposing otherwise poorly exposed epitopes that serve as highly potent targets for antibodies that inhibit binding of pathogenic proteins to host cell receptors.

A particular embodiment of the invention provides methods for inducing antibodies having enhanced ability to block binding of a parasitic ligand to its host cell receptor, by immunization with a mutant form of the parasitic ligand (i.e., having one or more amino acid modifications relative to the wild type or reference ligand), whereby the antibodies elicited by the mutant ligand have greater functional inhibitory activity than antibodies elicited by the wild-type or reference ligand. In particular embodiments, the parasitic ligand has one or more mutations relative to the wild type or reference parasitic ligand, which mutations result in exposing regions which are poorly exposed to solvent and/or poorly accessible for antibody production in vivo in the wild type ligand.

Highly preferred embodiments of the invention provide methods for inducing antibodies having enhanced ability to block binding of a microbial adhesin protein to its host cell receptor, by immunization with a mutant form of the adhesin protein, which mutants induce of antibodies with greater inhibitory activity than antibodies elicited by the wild-type adhesin protein. In particular embodiments, the adhesin protein has one or more mutations relative to the wild type or a reference adhesin, which mutations result in exposing regions

of the protein which are poorly exposed in the wild type protein. In other embodiments, the mutations significantly reduce or abolish binding of the adhesin to its host cell surface receptor.

5

10

15

20

25

30

35

Accordingly, the present invention also relates to antibodies that target protein binding interactions including but not limited to examples such as antibodies that target $\alpha V \beta 3$ integrin, FimH, FimCH, and RSV. Embodiments provide antibodies that immunospecifically bind a member of a binding pair. The binding pair can be any two molecules that specifically interact with each other. In specific embodiments, the one member of the binding pair is an antigen of an infectious disease agent (*i.e.*, a molecule on the surface of an infectious disease agent) or a cellular receptor for an infectious disease agent. Such antigens of infectious disease agents include FimH of *E. coli*, and antigens of HSV-2, gonococcus, *Treponema pallidum*, *Chlamydia trachomatis* or human papillomavirus The first member of the binding pair can also be a cancer antigen (*i.e.*, a molecule expressed on the surface of a cancer cell). Such cancer antigens include human milk fat globule antigen (HMFG), an epitope of polymorphic epithelial mucin antigen (PEM), or a human colon carcinoma-associated protein antigen.

The invention further provides methods of treatment or prevention using the antibodies of the invention as discussed herein. For example, peptides to elicit antibodies or antibodies directed to an infectious agent or a cellular receptor for an infectious disease agent or a cancer antigen can be used in the treatment or prevention of an infectious disease or a cancer associated with the expression of the particular antigen of the infectious disease agent or the cellular receptor for the infectious disease agent.

In a preferred embodiment of the invention, antibodies to mutant adhesin proteins are generated to inhibit binding of adhesins to cellular receptors. In particular, FimH proteins are responsible for the adhesin binding of type 1 pili to bladder epithelial cells. Accordingly, the invention provides mutant forms of FimH (relative to the FimH amino acid sequence of Figure 1 (SEQ ID NO:3) or corresponding FimH variant of Figure 3) or other bacterial adhesin (e.g., PapG) that elicit antibodies that have greater inhibitory activity (that prevents binding of the bacteria or the isolated adhesin to the cellular receptor (mannose moieties in the case of FimH) or host cell (bladder epithelial cells in the case of FimH) than antibodies elicited by wild type or a reference FimH or other bacterial adhesin. Without being limited by theory, the invention provides mutant forms of FimH in which the canyon region of FimH, which is involved in mannose binding, adopts a more open conformation, exposing regions that are poorly exposed in wild type FimH. FimH residues involved in maintaining the canyon structure and/or that, when mutated, would result in

exposing poorly exposed regions in the wild type FimH may be identified by any method known in the art. For example, such residues may be identified by protein modeling. The crystal structure for the FimCH complex is depicted in Choudhury et al., 1999, *Science* 285:1061-1066, which is hereby incorporated by reference in its entirety. More importantly, the crystal structure of the mannose binding pocket of FimH has been determined by co-crystallizing a highly purified FimCH chaperone-adhesin complex together with D-mannose (see Figure 2).

In other embodiments, mutant FimH proteins, or other bacterial adhesins, are provided where one or more amino acid modifications are introduced into the FimH protein that significantly reduce or abolish binding of FimH to mannose or the other bacterial adhesin to its cell surface receptor. In either embodiment, the residues to be modified may be identified through protein modeling and/or analysis of site specific or naturally occurring or any other mutants to identify residues that, when mutated, alter protein structure or binding of the protein to its cellular receptor. In certain embodiments, libraries of mutant adhesins having random mutations at one or more residues are screened for mutant adhesins in which poorly exposed mutant regions are exposed, mutant adhesins that lack or have significantly reduced binding to the cellular receptor, and/or mutant adhesins that can elicit antibodies that have greater functional inhibitory activity than antibodies elicited by the wild type or reference adhesin.

20

25

30

35

5

10

15

In preferred embodiments, the mutant protein of the invention is a mutant FimH protein having one or more amino acid modifications (preferably substitutions) at one or more of residues 1, 2, 3, 4, 10, 11, 12, 13, 14, 15, 16, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 77, 78, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145 or 146 of the FimH amino acid sequence in Figure 1 (SEQ ID NO:3) (the residue numbers discussed herein all refer to the residues as numbered on the FimH sequence of Figure 1, unless specifically noted and intend to include corresponding residues in a variant of FimH, as determined by sequence alignment with the amino acid sequence in Figure 1). In a more preferred embodiment, the amino acid modifications (preferably substitutions) are made at one or more of residues 1, 2, 13, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 77, 78, 101, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143 or 144 of the amino acid sequence of FimH in Figure 1 (SEQ ID NO:3). In yet another embodiment, the amino acid modifications (preferably substitutions) are made at one or more of residues 1, 45, 46, 47, 52, 53, 54, 55, 56, 93, 94, 95, 133, 134 or 135 of the amino acid sequence of FimH (Figure 1). In another embodiment, the amino acid modifications (preferably

substitutions) are made at one or more of residues 1, 3, 44, 54, 133, 135, 140, 142 and 144 of the amino acid sequence of FimH (Figure 1). In a preferred embodiment, the amino acid modification (preferably substitution) is at residue 54, 133, or 135 of the amino acid sequence of FimH (Figure 1), more preferably where the residue at position 54, 133, or 135 is substituted with a charged residue (in other embodiments substituted with an amino acid having greater steric effects than the wild type residue). In more preferred embodiments, the amino acid residue at position 54 can be substituted with asparagine or alanine; the residue at amino acid position 133 can be substituted with lysine, arginine, glutamate, or histidine; and/or the amino acid residue at position 135 can be substituted with aspartic acid. In other embodiments, the FimH amino acid modifications are in canyon region of FimH, preferably where the canyon region has a surface of residues 1, 13, 46, 47, 48, 52, 54, 133, 135, 137, 138, 140 and 142.

In one embodiment, the site of one or more of the amino acid modifications occurs at a residue that interacts with mannose e.g., as determined by molecular modeling using the crystal structure provided in Figure 2, or the crystal structure in Choudhury et al. 1999, (Science 285:1061-1066, incorporated by reference herein in its entirety) or both. Further, the mutations can similarly be made by modeling based upon related crystal structures such as that disclosed herein as Figure 2 and in application no. 09/637,216 filed August 11, 2000, entitled "Anti-Bacterial Compounds Directed vs Pilus Biogenesis, Adhesion and Activity; Co-crystals of Pilus Subunits and Methods of Use" by Hultgren et al., which is herein incorporated by reference.

For example, the modification is made at one or more residues 1, 46, 47, 54, 133, 135, 140, and 142 of FimH (SEQ ID NO:3), which interact with mannose as shown in Table 1.

25

30

20

5

10

15

Table 1: FimH Amino Acid Residues Which Interact with Mannose

residue position	amino acid residue
1	phenylalanine (F)
46	asparagine (N)
47	aspartic acid (D)
54	aspartic acid (D)
133	glutamine (Q)
135	asparagine (N)

140	aspartic acid (D)
142	phenylalanine (F)

In another embodiment, the site of one or more of the amino acid modifications occurs within the hydrophobic ring surrounding the mannose-binding pocket of FimH. For example, residues 13, 48, 52, and 142 of FimH (SEQ ID NO:3), as shown in Table 2.

Table 2: FimH Amino Acid Residues of the Hydrophobic Ring

residue position	amino acid residue
13	isoleucine (I)
48	tyrosine (Y)
52	isoleucine (I)
142	phenylalanine (F)

In one embodiment, the site of one or more of the amino acid modifications occurs within about 15 angstroms from the a carbon residue 54 of FimH, e.g., as determined by molecular modeling using the crystal structure provided in Figure 2 and in Choudhury et al. 1999, (Science 285:1061-1066, incorporated by reference herein in its entirety). For example, the modification is made at one or more residues 1, 2, 3, 4, 10, 11, 12, 13, 14, 15, 16, 42, 43, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 58, 59, 77, 78, 89, 90, 91, 92, 93, 94, 95, 96, 97, 98, 99, 100, 101, 102, 103, 104, 105, 130, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143, 144, 145 and 146 of FimH (SEQ ID NO:3). (see Table 3)

Table 3: Residues 15 angstroms from the α carbon of residue 54 in FimH

	residue position	wild type amino acid
30	1	phenylalanine (F)
	2	alanine (A)
	3	cysteine (C)
	4	lysine (K)
35	10	alanine (A)

5

10

15

20

25

	11	isoleucine (I)
	12	proline (P)
5	13	isoleucine (I)
	14	glycine (G)
	15	glycine (G)
	16	glycine (G)
	42	isoleucine (I)
10	43	phenylalanine (F)
	44	cysteine (C)
	45	histidine (H)
	46	asparagine (N)
15	47	aspartic acid (D)
	48	tyrosine (Y)
	49	proline (P)
	50	glutamic acid (E)
20	51	asparagine (N)
	52	isoleucine (I)
	53	threonine (T)
	54	aspartic acid (D)
25	55	tyrosine (Y)
23	56	valine (V)
	57	threonine (T)
30	58	leucine (L)
	59	glutamine (Q)
	78	serine (S)
	89	glutamic acid (E)
	90 .	threonine (T)
	91	proline (P)
35	92	arginine (R)

	93	valine (V)
	94	valine (V)
5	95	tyrosine (Y)
	96	asparagine (N)
	97	serine (S)
	98	arginine (R)
	99	threonine (T)
10	101	lysine (K)
	102	proline (P)
	103	tryptophan (W)
	104	proline (P)
15	105	valine (V)
	130	isoleucine (I)
	131	leucine (L)
	132	arginine (R)
20	133	glutamine (Q)
	134	threonine (T)
	135	asparagine (N)
	136	asparagine (N)
25	137	tyrosine (Y)
23	138	asparagine (N)
	139	serine (S)
30	140	aspartic acid (D)
	141	aspartic acid (D)
	142	phenylalanine (F)
	143	glutamine (Q)
	144	phenylalanine (F)
	145	valine (V)
35	146	tryptophan (W)

In another embodiment, the site of one or more of the amino acid modifications occurs within about 10 angstroms from the α carbon residue 54 of FimH. For example, residues 1, 2, 13, 44, 45, 46, 47, 48, 49, 50, 51, 52, 53, 54, 55, 56, 57, 77, 78, 101, 131, 132, 133, 134, 135, 136, 137, 138, 139, 140, 141, 142, 143 and 144 of FimH (SEQ ID NO:3) (see Table 4)

Table 4: Residues 10 angstroms from the α carbon of residue 54 in FimH

	residue position	wild type amino acid
10	1	phenylalanine (F)
	2	alanine (A)
	13	isoleucine (I)
	44	cysteine (C)
15	45	histidine (H)
	46	asparagine (N)
	47	aspartic acid (D)
٠	48	tyrosine (Y)
20	49	proline (P)
20	50	glutamic acid (E)
	51	asparagine (N)
	52	isoleucine (I)
	53	threonine (T)
25	54	aspartic acid (D)
	55	tyrosine (Y)
	56	valine (V)
30	57	threonine (T)
	91	proline (P)
	92	arginine (R)
	93	valine (V)
	94	valine (V)
35	95	tyrosine (Y)

5

96	asparagine (N)
97	serine (S)
98	arginine (R)
99	threonine (T)
101	lysine (K)
131	leucine (L)
132	arginine (R)
133	glutamine (Q)
134	threonine (T)
135	asparagine (N)
136	asparagine (N)
137	tyrosine (Y)
138	asparagine (N)
139	serine (S)
140	aspartic acid (D)
141	aspartic acid (D)
142	phenylalanine (F)
143	glutamine (Q)
144	phenylalanine (F)
	97 98 99 101 131 132 133 134 135 136 137 138 139 140 141 142 143

In another embodiment, the site of one or more of the amino acid modifications occurs within about 5 angstroms from the α carbon of residue 54 of FimH. For example, the modification is at one or more of residues 1, 45, 46, 47, 52, 53, 54, 55, 56, 93, 94, 95, 133, 134 and 135 of FimH (SEQ ID NO:3). (see Table 5)

30 Table 5: Residues 5 angstroms from the α carbon of residue 54 in FimH

residue position	wild type amino acid
1	phenylalanine (F)
45	histidine (H)
46	asparagine (N)

35

47	aspartic acid (D)
52	isoleucine (I)
53	threonine (T)
54	aspartic acid (D)
55	tyrosine (Y)
56	valine (V)
93	valine (V)
94	valine (V)
95	tyrosine (Y)
133	glutamine (Q)
134	threonine (T)
135	asparagine (N)
	52 53 54 55 56 93 94 95 133 134

In another embodiment, the amino acid modifications are made within 15, 10 and 5 angstroms of the α -carbon of residues 1, 13, 46, 47 48, 54, 133, 135, 140 or 142 of the FimH binding domain.

20

25

5.2 PROPHYLACTIC AND THERAPEUTIC USES

The present invention encompasses methods of treatment and prophylaxis and therapies which involve administering mutant proteins or polypeptides to an animal, preferably a mammal, and most preferably a human, for preventing, treating, or ameliorating symptoms associated with a disease, disorder, or infection. Prophylactic and therapeutic compounds of the invention include, but are not limited to, mutant proteins, polypeptides, antibodies elicited by the mutant proteins and polypeptides and nucleic acids encoding the proteins and antibodies. Proteins and antibodies may be provided in pharmaceutically acceptable compositions as known in the art or as described herein.

30

35

Methods of the invention include methods of treatment and prophylaxis involving administration of a mutant polypeptide or protein of the invention that elicits high potency inhibitory antibodies that inhibit or reduce protein binding, particularly where the protein binding is relevant to some disease or disorder. For example, peptides which elicit antibodies and the resulting antibodies which disrupt or prevent the interaction between an antigen and its binding partner may be administered to an animal, preferably a mammal and

most preferably a human, to treat, prevent or ameliorate one or more symptoms associated with infection.

In a specific embodiment, the methods of the invention produce antibodies that prevent a viral or bacterial antigen from binding to its binding partner (e.g., host cell receptor) by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 45%, at least 45%, at least 35%, at least 25%, at least 20%, or at least 10% relative to antigen binding to its host cell receptor in the absence of said antibodies.

Peptides and proteins that elicit antibodies which do not prevent a viral or bacterial antigen from binding its host cell receptor but inhibit or downregulate viral or bacterial replication can also be administered to an animal to treat, prevent or ameliorate one or more symptoms associated with a viral or bacterial infection. The ability of an antibody to inhibit or downregulate viral or bacterial replication may be determined by techniques described herein or otherwise known in the art. For example, the inhibition or downregulation of viral replication can be determined by detecting the viral titer in the animal.

Examples of pathogen host cell receptor interactions that may be disrupted in methods of the invention include, but are not limited to, those in Table 6.

Table 6

5

Pathogen	Cellular Receptor
B-lymphotropic papovavirus (LAV)	LAV receptor on B-cells
Bordetella pertussis	Adenylate cyclase
Borna Disease virus (BDV)	BDV surface glycoproteins
Bovine coronavirus	N-acetyl-9-O-acetylneuraminic acid receptor
Choriomeningitis virus	CD4+
Dengue virus	Highly sulphated type Heparin sulphate p65
E. coli	Galα(1-4)Gal-containing receptors mannose-containing receptors
Ebola	CD16b

25

30

	Pathogen	Cellular Receptor
	Echovirus 1	Integrin VLA-2 receptor
5	Echovirus-11 (EV)	EV receptor
	Endotoxin (LPS)	CD14
	Enteric bacteria	Glycoconjugate receptors
	Enteric Orphan virus	alpha/beta T-cell receptor
	Enteroviruses	Decay-accelerating factor receptor
10	Feline leukemia virus	Extracellular envelope glycoprotein (Env-SU) receptor
	Foot and mouth disease virus	Immunoglobulin Fc receptorPoxvirusM-T7
	Gibbon ape leukemia virus (GALV)	GALV receptor
15	Gram-negative bacteria	CD14 receptor
15	Heliobacter pylori	Lewis(b) blood group antigen receptor
	Hepatitis B virus (HBV)	T-cell receptor
	Herpes Simplex Virus	Heparin sulphate glycoaminoglycan receptor
		Fibroblast growth factor receptor
20	HIV-1	CC-Chemokine receptor CCR5
		CD11a
		CD2
		G-protein coupled receptor
25		CD4
23	Human cytomegalovirus	Heparin sulphate proteoglycan
		Annexin II
		CD13 (aminopeptidase N)
	Human coronovirus	Human aminopeptidase N receptor
30	Influenza A, B & C	Hemagglutinin receptor
	Legionella	CR3 receptor
*		Protein kinase receptor
		Galactose N-acetylgalactosamine (Gal/GalNAc)-
	·	inhibitable lectin receptor
35		Chemokine receptor

	Pathogen	Cellular Receptor
	Leishmania mexicana	Annexin I
	Listeria monocytogenes	ActA protein
5	Measles virus	CD46 receptor
	Meningococcus	Meningococcal virulence associated Opa receptors
	Morbilliviruses	CD46 receptor
10	Mouse hepatitis virus	Carcinoembryonic antigen family receptors Carcinoembryonic antigen family Bg1a receptor
	Murine leukemia virus	Envelope glycoproteins
	Murine gamma herpes virus	gamma interferon receptor
	Murine retrovirus	Glycoprotein gp70 Rmc-1 receptor
15	Murine coronavirus mouse hepatitis virus	Carcinoembryonic antigen family receptors
	Mycobacterium avium-M	Human Integrin receptor alpha v beta 3
20	Neisseria gonorrhoeae	Heparin sulphate proteoglycan receptor CD66 receptor Integrin receptor Membrane cofactor protein CD46
25		GM1 GM2 GM3 CD3 Ceramide
30	Newcastle disease virus	Hemagglutinin-neuraminidase protein Fusion protein
	Parvovirus B19	Erythrocyte P antigen receptor
i	Plasmodium falciparum	CD36 receptor Glycophorin A receptor
35	Pox Virus	Interferon gamma receptor

- 39 -

Pathogen	Cellular Receptor
Pseudomonas	KDEL receptor
Rotavirus	Mucosal homing alpha4beta7 receptor
Samonella typhiurium	Epidermal growth factor receptor
Shigella	α5β1 integrin protein
Streptococci	Nonglycosylated J774 receptor
T-helper cells type 1	Chemokine receptors including: CXCR1-4 CCR1-5 CXCR3
T-cell lymphotropic virus 1	gp46 surface glycoprotein
Vaccinia virus	TNFRp55 receptor TNFRp75 receptor Soluble Interleukin-1 β receptor

20

25

35

15

5

10

In a specific embodiment, an antibody inhibits or downregulates viral or bacterial replication by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 40%, at least 45%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to viral or bacterial replication in absence of said antibody.

Proteins and peptides that elicit antibodies and the resulting antibodies can also be used to prevent, inhibit or reduce the growth or metastasis of cancerous cells. In a specific embodiment, an antibody inhibits or reduces the growth or metastasis of cancerous cells by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 45%, at least 45%, at least 45%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to the growth or metastasis in absence of said antibody. Examples of cancers include, but are not limited to, leukemia (e.g., acute leukemia such as acute lymphocytic leukemia and acute myelocytic leukemia), neoplasms, tumors (e.g., fibrosarcoma, myxosarcoma, liposarcoma, chondrosarcoma, osteogenic sarcoma, chordoma, angiosarcoma, endotheliosarcoma, lymphangiosarcoma,

lymphangioendotheliosarcoma, synovioma, mesothelioma, Ewing's tumor, leiomyosarcoma, rhabdomyosarcoma, colon carcinoma, pancreatic cancer, breast cancer, ovarian cancer, prostate cancer, squamous cell carcinoma, basal cell carcinoma, adenocarcinoma, sweat gland carcinoma, sebaceous gland carcinoma, papillary carcinoma, papillary adenocarcinomas, cystadenocarcinoma, medullary carcinoma, bronchogenic carcinoma, renal cell carcinoma, hepatoma, bile duct carcinoma, choriocarcinoma, seminoma, embryonal carcinoma, Wilms' tumor, cervical cancer, testicular tumor, lung carcinoma, small cell lung carcinoma, bladder carcinoma, epithelial carcinoma, glioma, astrocytoma, medulloblastoma, craniopharyngioma, ependymoma, pinealoma, hemangioblastoma, acoustic neuroma, oligodendroglioma, meningioma, melanoma, neuroblastoma, and retinoblastoma), heavy chain disease, metastases, or any disease or disorder characterized by uncontrolled cell growth.

5

10

15

20

25

30

35

Proteins and peptides that elicit antibodies and antibodies can also be used to reduce the inflammation experienced by animals, particularly mammals, with inflammatory disorders. In a specific embodiment, an antibody reduces the inflammation in an animal by at least 99%, at least 95%, at least 90%, at least 85%, at least 80%, at least 75%, at least 75%, at least 75%, at least 30%, at least 45%, at least 45%, at least 45%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to the inflammation in an animal in the not administered said protein, peptide or antibody. Examples of inflammatory disorders include, but are not limited to, rheumatoid arthritis and asthma.

Peptides, proteins and antibodies of the invention can also be used to prevent the rejection of transplants. Antibodies can also be used to prevent clot formation. Further, peptides and proteins that elicit antibodies and antibodies that function as agonists of the immune response can also be administered to an animal, preferably a mammal, and most preferably a human, to treat, prevent or ameliorate one or more symptoms associated with the disease, disorder, or infection.

The compositions of this invention may also be advantageously utilized in combination with other monoclonal or chimeric antibodies, or with lymphokines or hematopoietic growth factors (such as, e.g., IL-2, IL-3, IL-7, and IL-9), which, for example, serve to increase the number or activity of effector cells which interact with the antibodies. The antibodies of this invention may also be advantageously utilized in combination with other monoclonal or chimeric antibodies, or with lymphokines or hematopoietic growth factors (such as, e.g., IL-2, IL-3, IL-7, and IL-9), which, for example, serve to increase the immune response. The compositions of this invention may also be advantageously utilized in combination with one or more drugs used to treat a disease, disorder, or infection such as,

for example anti-cancer agents, anti-inflammatory agents anti-viral agents, or antibiotics. Examples of anti-cancer agents include, but are not limited to, isplatin, ifosfamide, paclitaxel, taxanes, topoisomerase I inhibitors (e.g., CPT-11, topotecan, 9-AC, and GG-211), gemcitabine, cisplatin, doxinedria, vinorelbine, oxaliplatin, 5-fluorouracil (5-FU), 5 leucovorin, vinorelbine, temodal, and taxol. Examples of anti-viral agents include, but are not limited to, cytokines (e.g., IFN-α, IFN-β, IFN-γ), inhibitors of reverse transcriptase (e.g., AZT, 3TC, D4T, ddC, ddI, d4T, 3TC, adefovir, efavirenz, delavirdine, nevirapine, abacavir, and other dideoxynucleosides or dideoxyfluoronucleosides), inhibitors of viral mRNA capping, such as ribavirin, inhibitors of proteases such HIV protease inhibitors (e.g., 10 amprenavir, indinavir, nelfinavir, ritonavir, and saquinavir,), amphotericin B, castanospermine as an inhibitor of glycoprotein processing, inhibitors of neuraminidase such as influenza virus neuraminidase inhibitors (e.g., zanamivir and oseltamivir), topoisomerase I inhibitors (e.g., camptothecins and analogs thereof), amantadine, and rimantadine. Examples of anti-inflammatory agents include, but are not limited to, nonsteroidal 15 anti-inflammatory drugs such as COX-2 inhibitors (e.g., meloxicam, celecoxib, rofecoxib, flosulide, and SC-58635, and MK-966), ibuprofen and indomethacin, and steroids (e.g., deflazacort, dexamethasone and methylprednisolone).

In a specific embodiment, antibodies administered to an animal are of a species origin or species reactivity that is the same species as that of the animal. Thus, in a preferred embodiment, human or humanized antibodies, or nucleic acids encoding human or human, are administered to a human patient for therapy or prophylaxis.

20

25

30

35

In a preferred embodiment, the present invention encompasses the administration of a mutant bacterial adhesin protein or fragment thereof, preferably associated with a pathogenic bacteria. The mutant bacterial adhesin protein is preferably a type 1 pilus polypeptide. Fragments of the bacterial adhesin protein containing, for example, all or an immunogenic portion of the mutant attachment domain (preferably, a portion that binds cell surface residues and/or mannose) of the protein may also be administered. Such bacterial adhesin proteins also include analogs, homologs and variants thereof, preferably that retain decrease binding activity. In other embodiments, the mutant bacterial adhesin proteins are provided as part of a complex, for example, with a bacterial chaperone protein, as detailed below.

In preferred embodiments, the methods of the invention encompass administration of a mutant FimH protein, including variants, derivatives, analogs and fragments thereof, preferably variants, derivatives, analogs and fragments that have decreased mannose binding activity and, preferably, are immunogenic. In one embodiment

of the present invention, recombinantly produced mutant FimH proteins (as well as functional analogs) from bacteria that produce type 1 pili are contemplated.

5

35

In additional preferred embodiments, the methods of the invention encompass administration of an antibody or antigen binding fragment thereof directed to the mutant proteins that have inhibitory functions with respect to the infective properties of the pathogen (e.g., prevent binding of the pathogen to its cellular receptor). In one embodiment of the present invention, recombinantly produced antibodies are contemplated.

In preferred embodiments, the invention provides methods of treating or preventing a bacterial infection, particularly a urogenital tract infection, more particularly a UTI, caused by a gram negative bacterium of the family Enterobacteriaceae, especially E. coli. In other embodiments, the infection is caused by Staphylococcus saprophyticus or Staphylococcus aureus, Klebsiella spp, Proteus spp, Serratia spp, or Pseudomonas spp. In an alternative embodiment, the infection is caused by infection with unusual organisms such as parasites, e.g., Echinococcus, Schistosoma haematobium or mansoni, protozoa, e.g.,

Trichomonas, yeast such as Candida spp, Blastomyces spp, or Coccidioides immitis, or acid-fast organisms such as Mycobacterium tuberculosis. In preferred embodiments, the infection to be treated or prevented using the methods of the invention is a UTI, a bladder infection, a kidney infection, pyelonephritis, cystitis, and asymptomatic bacteriuria.

In one embodiment, the primate is a human. In another embodiment, the 20 human subject is susceptible to a recurrence of UTI due to having had a prior UTI, particularly having had two, three or even more UTIs in one year, or has a familial susceptibility, e.g., genetic predisposition. In other embodiments, the human subject is pregnant and/or hospitalized, or is immuno-compromised due, for example, to a secondary disease, such as HIV or cancer, or having undergone therapies therefor, has an HIV infection 25 or has a cancer, or is in remission therefrom. In a specific embodiment, the human subject has asymptomatic bactourea and, in particular embodiments, also is diabetic and/or is a pregnant woman. Reduced levels of IL-6 and/or IL-8 as compared to the normal levels of IL-6 and IL-8 in pregnant women have been correlated with difficulty in clearing urinary tract infections. Thus, the invention further includes treatment of pregnant women with 30 reduced levels of IL-6 and/or IL-8. In another specific embodiment, the subject is at risk of developing end stage renal disease; accordingly, the invention further provides a method for preventing progression to end stage renal disease.

In a preferred embodiment, the compositions of the invention are administered parenterally, preferably via intramuscular, intravenous or subcutaneous injection; orally; transdermally; muscosally, including vaginally, rectally, buccally,

preferably the mucosal delivery is via a vaginal suppository; and finally via pulmonary delivery. Preferably, the compositions are not injected intraperitoneally.

5

10

15

20

25

30

35

The polypeptides and antibodies of the present invention may also be present in the form of a composition. Such compositions, where used for pharmaceutical purposes, will commonly have the polypeptide of the present invention suspended in a pharmacologically acceptable diluent or excipient, or they may be in lyophilized form. The methods of the invention encompass administering an effective amount of composition to elicit sufficient levels of antibodies, particularly IgGs, in serum and, preferably, in mucosal secretions, such as urine and/or genital secretions, to prevent bacterial infection, e.g., to reduce the incidence of such bacterial infections, or to treat or ameliorate the symptoms of bacterial infection.

5.3 PHARMACEUTICAL FORMULATIONS AND ADMINISTRATION OF MUTANT PROTEINS

The mutant polypeptides and fragments thereof described herein are useful immunogens for preparing pharmaceutical compositions that stimulate the production of antibodies that inhibit the interaction of binding partners. This antibody inhibition is greater than that of antibodies raised against the corresponding non-mutant polypeptides.

The antibodies of the invention can be directed to any protein that has a binding partner. In preferred embodiments, the antibodies have enhanced functional inhibitory activity to block binding of a pathogenic protein to its host cell receptor. A particular embodiment of the invention provides antibodies having enhanced ability to block binding of a parasitic ligand to its host cell receptor. Highly preferred embodiments of the invention provide antibodies having enhanced ability to block binding of a microbial adhesin protein to its host cell receptor. In the most preferred embodiment, the microbial adhesion protein is FimH.

The pharmaceutical compositions useful herein also contain a pharmaceutically acceptable carrier, including any suitable diluent or excipient, which includes any pharmaceutical agent that does not itself induce the production of antibodies harmful to the primate receiving the composition, and which may be administered without undue toxicity.

In preferred embodiments, the pharmaceutical formulations of the invention comprise a FimH polypeptide (preferably, mutant FimH polypeptide of the invention), FimCH polypeptide complex (preferably where the FimH component is a mutant FimH of the invention) or fragments or variants thereof, and a pharmaceutically acceptable carrier or

excipient. Pharmaceutically acceptable carriers include but are not limited to saline, buffered saline, dextrose, water, glycerol, sterile isotonic aqueous buffer, and combinations thereof. A thorough discussion of pharmaceutically acceptable carriers, diluents, and other excipients is presented in *Remington's Pharmaceutical Sciences* (Mack Pub. Co., N.J. current edition). The formulation should suit the mode of administration. In a preferred embodiment, the formulation is suitable for administration to humans, preferably is sterile, non-particulate and/or non-pyrogenic. In a preferred embodiment the pharmaceutical composition contains a citrate buffer, preferably, about 20 mM sodium citrate and 0.2 M NaCl, more preferably with a pH of 6.0, and an adjuvant, such as MF59C.1 (Chiron, Emeryville, CA).

5

10

15

25

30

35

The composition, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents. The composition can be a solid form, such as a lyophilized powder suitable for reconstitution, a liquid solution, suspension, emulsion, tablet, pill, capsule, sustained release formulation, or powder. Oral formulation can include standard carriers such as pharmaceutical grades of mannitol, lactose, starch, magnesium stearate, sodium saccharine, cellulose, magnesium carbonate, etc.

Generally, the ingredients are supplied either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachette indicating the quantity of active agent. Where the composition is administered by injection, an ampoule of sterile diluent can be provided so that the ingredients may be mixed prior to administration.

The invention provides in one embodiment a thermally stable and/or chemically stable pharmaceutical composition that is suitable for reconstitution into an injectable sterile and particulate-free solution.

The invention also provides a pharmaceutical pack or kit comprising one or more containers filled with one or more of the ingredients of the vaccine formulations of the invention. In a preferred embodiment, the kit comprises two containers, one containing the adhesin protein or protein complex and the other containing an adjuvant. Associated with such container(s) can be a notice in the form prescribed by a governmental agency regulating the manufacture, use or sale of pharmaceuticals or biological products, which notice reflects approval by the agency of manufacture, use or sale for human administration.

The invention also provides that mutant polypeptide, or polypeptide complex or fragments thereof are packaged in a hermetically sealed container such as an ampoule or sachette indicating the quantity of composition. In one embodiment, the composition is supplied as a liquid, in another embodiment, as a dry sterilized lyophilized powder or water

free concentrate in a hermetically sealed container and can be reconstituted, e.g., with water or saline to the appropriate concentration for administration to a subject. Preferably, the composition is supplied as a dry sterile lyophilized powder in a hermetically sealed container at a unit dosage of preferably, 1 μ g, 5 μ g, 10 μ g, 20 μ g, 25 μ g, 30 μ g, 50 μ g, 75 μ g, 100 μ g, 123 μ g, 150 μ g, or 200 μ g. Alternatively, the unit dosage of the composition is less than 1 μ g, (for example 0.5 μ g or less, 0.25 μ g or less, or 0.1 μ g or less), or more than 123 μ g, (for example 150 μ g or more, 250 μ g or more, or 500 μ g or more).

5

10

15

20

25

30

35

The composition should be administered within 12 hours, preferably within 6 hours, within 5 hours, within 3 hours, or within 1 hour after being reconstituted from the lyophylized powder.

In an alternative embodiment, a mutant polypeptide or fragment thereof is supplied in liquid form in a hermetically sealed container indicating the quantity and concentration of the polypeptide composition. Preferably, the liquid form of the mutant polypeptide or fragment thereof is supplied in a hermetically sealed container at least 50 μ g/ml, more preferably at least 100 μ g/ml, at least 200 μ g/ml, at least 500 μ g/ml, at least 1 mg/ml, and most preferably 490 μ g/ml.

In a preferred embodiment, mutant polypeptide is stored in a 3 ml sterile vial containing 1.0 ml of vaccine formulated in 500 µg/ml of mutant polypeptide in 20 mM sodium citrate, 0.2 M NaCl at a pH of 6.0. In this formulation, the vial should contain a clear colorless liquid. The adjuvant is stored in a separate 3 ml vial containing 0.7 ml of adjuvant (MF59C.1; 39 mg/ml squalene, 4.7 mg/ml each Tween 80 and Span 85, 10 mM citrate in sterile water for injection at pH 6.5) and is typically a cloudy, white, turbid liquid. The diluent is supplied in another separate 3 ml vial containing 2.0 ml of 20 mM sodium citrate, 0.2 M NaCl at a pH of 6.0. The diluent is a clear, colorless liquid. Each of these vials should be stored in a refrigerator (2°C to 8°C/36°F to 46°C).

In a preferred embodiment, the mutant polypeptide is prepared for injection into a subject immediately prior to the injection, i.e., mixed with diluent and adjuvant.

Doses of 1 μ g, 5 μ g, 25 μ g and 123 μ g of mutant polypeptide are preferably prepared for administration as follows:

For a 1µg dose, gently invert several times one mutant polypeptide vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.5 ml from the vaccine vial into a 1.0 ml syringe and inject into a diluent vial. Immediately mix by gently swirling. Withdraw 0.5 ml using a new needle and inject into a second diluent vial. Immediately mix by gently swirling. Withdraw 0.5 ml using a new needle and inject into the third diluent vial. Immediately mix by gently

swirling. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 1 µg of mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

5

35

For a 5 μg dose, gently invert several times one vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.5 ml using a new needle and inject into a second diluent vial. Immediately mix by gently swirling. Withdraw 0.5 ml using a new needle and inject into the third diluent vial. Immediately mix by gently swirling. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 5 μg of the mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

For a 25 μ g dose, gently invert several times one vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.5 ml using a new needle and inject into the third diluent vial. Immediately mix by gently swirling. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial.

Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 25 μg of the mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

For a 123 μ g dose, gently invert several times one vaccine vial, three diluent vials and one adjuvant vial and let stand at room temperature for twenty minutes. Withdraw 0.7 ml using a new needle and inject into the adjuvant vial. Immediately mix by gently inverting the vial 5-10 times. Withdraw 0.7 ml into a new 1.0 ml syringe using a new

needle. Disconnect the needle used to draw up the drug, attach a sterile 23 gauge, one inch needle for administration to the subject, and adjust the final volume in the syringe to 0.5 ml (eject any extra through the needle), label syringe and place in the labeled zip-lock bag. This 0.5 ml dose will contain approximately 123 µg of the mutant polypeptide and MF59C.1 (approximately 10 mg squalene) in 15 mM sodium citrate and 0.1 M NaCl.

In another specific embodiment, 1, 5, 25 or 123 µg of the mutant polypeptide in 0.5 ml of MF59C.1, as prepared above, is injected slowly, i.e., 20 to 30 seconds, into the deltoid muscle of the upper arm of the subject at day 0, followed by a booster dose approximately one month, and a second booster, if necessary approximately 4-6 months, after the initial administration. The necessity of booster shots can be determined by measuring serum, urine or mucosal secretions for immunoglobulins specific to the polypeptide injected.

5.3.1 <u>ADJUVANTS</u>

The invention encompasses mutant proteins e.g., FimH compositions, for use in vaccines administered in conjunction with adjuvants, wherein the adjuvants can be mixed (before or simultaneously upon injection) with the mutant polypeptide composition or

alternatively the adjuvant is not mixed with the mutant polypeptide composition but is

separately co-administered with the mutant polypeptide composition.

5

10

20

30

35

Mutant polypeptide compositions are administered with one or more adjuvants. In one embodiment, the mutant polypeptide composition is administered together with a mineral salt adjuvants or mineral salt gel adjuvant. Such mineral salt and mineral salt gel adjuvants include, but are not limited to, aluminum hydroxide (ALHYDROGEL, REHYDRAGEL), aluminum phosphate gel, aluminum hydroxyphosphate (ADJU-PHOS),

and calcium phosphate.

In another embodiment, the mutant polypeptide composition is administered with an immunostimulatory adjuvant. Such class of adjuvants, include, but are not limited to, cytokines (e.g., interleukin-2, interleukin-7, interleukin-12, granulocyte-macrophage colony stimulating factor (GM-CSF), interferon-γ, interleukin-1β (IL-1β), and IL-1β peptide or Sclavo Peptide), cytokine-containing liposomes, triterpenoid glycosides or saponins (e.g., QuilA and QS-21, also sold under the trademark STIMULON, ISCOPREP), Muramyl Dipeptide (MDP) derivatives, such as N-acetyl-muramyl-L-threonyl-D-isoglutamine (Threonyl-MDP, sold under the trademark TERMURTIDE), GMDP, N-acetyl-nor-muramyl-L-alanyl-D-isoglutamine, N-acetylmuramyl-L-alanyl-D-isoglutaminyl-L-alanine-2-(1'-2'-

dipalmitoyl-sn-glycero-3-hydroxyphosphoryloxy)-ethylamine, muramyl tripeptide

phosphatidylethanolamine (MTP-PE), unmethylated CpG dinucleotides and oligonucleotides, such as bacterial DNA and fragments thereof, LPS, monophosphoryl Lipid A (3D-MLAsold under the trademark MPL), and polyphosphazenes.

In another embodiment, the adjuvant used is a CpG adjuvant. Oligodeoxynucleotides (ODN) containing unmethylated CpG dinucleotides within specific sequence contexts (CpG motifs) are detected, like bacterial or viral DNA, as a danger signal by the vertebrate immune system. CpG ODN synthesized with a nuclease-resistant phosphorothioate backbone have been shown to be a potent Th1-directed adjuvant in mice. In addition, an ODN with a TpC dinucleotide at the 5' end followed by three 6 mer CpG motifs (5'-GTCGTT-3') separated by TpT dinucleotides has shown high immunostimulatory activity for human, chimpanzee, and rhesus monkey leukocytes (Hartmann et al., 2000, J. Immun, 164: 1617-1624).

5

10

15

20

25

30

35

In another embodiment, suitable adjuvants include, but are not limited to: aluminim hydroxide, N-acetyl-muramyl-L-threonyl-D-isoglutamine (thr-MDP), -acetyl-nor-muramyl-L-alanyl-D-isoglutamine, N-acetylmuramyl-L-alanyl-D-isoglutaminyl-L-alanine-2-(1'-2'-dipalmitoyl-sn-glycero-3-hydroxyphosphoryloxy)-ethylamine.

In another embodiment, the adjuvant used is a particulate adjuvant, including, but not limited to, emulsions, e.g., squalene or squaline oil-in-water adjuvant formulations, such as SAF and MF59, e.g., prepared with block-copolymers, such as L-121 (polyoxypropylene/polyoxyethylene) sold under the trademark PLURONIC L-121, Liposomes, Virosomes, cochleates, and immune stimulating complex, which is sold under the trademark ISCOM. In a preferred embodiment, the adjuvant is MF59, MF59C or most preferably MF59C.1 (Chiron, Emeryville, CA) or a derivative thereof. Freund's Complete Adjuvant and Freund's Incomplete Adjuvant are also commonly used adjuvants in test animals, however these adjuvants are less preferred in primates, in particular for use in humans.

In another embodiment, a microparticulate adjuvant is used. Microparticulate adjuvants include, but are not limited to biodegradable and biocompatible polyesters, homoand copolymers of lactic acid (PLA) and glycolic acid (PGA), poly(lactide-co-glycolides) (PLGA) microparticles, polymers that self-associate into particulates (poloxamer particles), soluble polymers (polyphosphazenes), and virus-like particles (VLPs) such as recombinant protein particulates, e.g., hepatitis B surface antigen (HbsAg).

Yet another class of adjuvants that may be used include mucosal adjuvants, including but not limited to heat-labile enterotoxin from *Escherichia coli* (LT), cholera holotoxin (CT) and cholera Toxin B Subunit (CTB) from *Vibrio cholerae*, mutant toxins

(e.g. LTK63 and LTR72), microparticles, and polymerized liposomes. Additional examples of mucous targeting adjuvants are *E. coli* mutant heat-labile toxin LT's with reduced toxicity, live attenuated organisms that bind M cells of the gastrointestinal tract, such as *V. cholera* and *Salmonella typhi*, *Mycobacterium bovis* (BCG), in addition to mucosal targeted particulate carriers such as phospholipid artificial membrane vesicles, copolymer microspheres, lipophilic immune-stimulating complexes and bacterial outer membrane protein preparations (proteosomes).

In other embodiments, any of the above classes of adjuvants may be used in combination with each other or with other adjuvants. For example, non-limiting examples of combination adjuvant preparations that can be used to administer the FimH compositions of the invention include liposomes containing immunostimulatory protein, cytokines, or T-cell and/or B-cell peptides, or microbes with or without entrapped IL-2 or microparticles containing enterotoxin. Other adjuvants known in the art are also included within the scope of the invention (*Vaccine Design: The Subunit and Adjuvant Approach*, Chap. 7, Michael F. Powell and Mark J. Newman (eds.), Plenum Press, New York, 1995, which is incorporated herein in its entirety).

The effectiveness of an adjuvant may be determined by measuring the induction of specific antibodies directed against the FimH composition formulated with the particular adjuvant. In a preferred embodiment, the adjuvant MF59C.1 is mixed with the vaccine composition, and MF59C.1 is at a dose of approximately 10 mg squalene, in 15 mM sodium citrate and 0.1 M NaCl.

25

20

5

10

15

30

35

5.3.2 VACCINE ADMINISTRATION

The invention provides methods of treatment, prophylaxis, and amelioration of one or more symptoms associated with pathogen infection by administering to a subject of an effective amount of a vaccine preparation comprising a protein of the invention or fragment thereof. The subject is preferably a mammal such as non-primate (e.g., cows, pigs, horses, cats, dogs, rats etc.) and a primate (e.g., monkey such as a cynomolgous monkey and a human). In a preferred embodiment, the subject is a human. In specific embodiments, the subject is a woman. The antibodies are particularly useful in women previously infected with UTI, pregnant women, and sexually active women. Finally, women previously infected with sexually transmitted diseases or otherwise at risk of UTI are recipients of the antibodies of the invention. In another embodiment, the subject is a diabetic, preferably a diabetic woman. In another embodiment, diabetic subjects can be vacciniated with WT FimCH.

5

10

15

20

25

30

35

Vaccines are generally administered parenterally using methods known in the art, however, many methods of administration may be used including but not limited to oral, intradermal, intramuscular, intravenous, subcutaneous, transdermal, intranasal routes, via pulmonary delivery, via suppository (e.g., vaginal suppository), via scarification (scratching through the top layers of skin, e.g., using a bifurcated needle). In a preferred embodiment, the vaccine is administered intramuscularly. In yet another embodiment, administration is not intraperitoneal due to the substantial risks of first pass hepatic removal of the polypeptides and also because of risk of infection and adhesions.

Various delivery vehicles are known and can be used to administer the mutant polypeptide compositions of the invention or fragments thereof, e.g., encapsulation in liposomes, microparticles, microcapsules, recombinant cells capable of expressing the mutant polypeptide compositions, receptor-mediated endocytosis (see, e.g., Wu and Wu, 1987, J. Biol. Chem. 262:4429-4432), construction of a nucleic acid as part of a retroviral or other vector, for example, the pCGA139-1-1 vector as described herein which can be administered as a DNA vaccine or alternatively, the nucleic acid vector can be introduced into a host cell such that the host cell expresses and secretes the vaccine composition, e.g., the mutant polypeptide complex, and the host cell is subsequently implanted into the subject contained within a membrane suitable for human implantation.

Methods of administering a polypeptide or fragment thereof, or pharmaceutical composition include, but are not limited to, parenteral administration (e.g., intradermal, intramuscular, intravenous and subcutaneous), epidural, mucosal (e.g., intranasal and oral or pulmonary routes or by vaginal suppositories), and topically. In a specific embodiment, compositions of the present invention or fragments thereof are

administered intramuscularly, intravenously, subcutaneously, or transdermally. The compositions may be administered by any convenient route, for example by infusion or bolus injection, by absorption through epithelial or mucocutaneous linings (e.g., oral mucous, colon, conjunctiva, nasopharynx, oropharynx, vagina, urethra, urinary bladder and intestinal mucosa, etc.) and may be administered together with other biologically active agents. Administration can be systemic or local.

5

10

15

20

25

In yet another embodiment, the vaccine composition is administered in such a manner as to target mucous tissues in order to elicit an immune response at the site of immunization. For example, mucosa tissues such as gut associated lymphoid tissue (GALT) can be targeted for immunization by using oral administration of compositions which contain adjuvants with particular mucosa targeting properties. Additional mucosal tissues can also be targeted, such as nasopharyngeal lymphoid tissue (NALT) and bronchial-associated lymphoid tissue (BALT) (Langermann, 1996, Seminars in Gast. Dis., 7:12-18); Wizemann et al., 1999, Emerging Inf. Dis., 5:395-403; Service, 1994, Science, 265:1522-1524).

In a specific embodiment, it may be desirable to administer the pharmaceutical compositions of the invention locally to the area in need of treatment; this may be achieved by, for example, and not by way of limitation, local infusion, by injection, or by means of an implant, said implant being of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes, or fibers. Preferably, when administering a an antibody of the invention or fragment thereof, care must be taken to use materials to which the FimH compositions does not absorb.

In another embodiment, the composition can be delivered in a vesicle, in particular a liposome (Langer, 1990, Science 249:1527-1533); Treat et al., 1989, in Liposomes in the Therapy of Infectious Disease and Cancer, Lopez-Berestein and Fidler (eds.), Liss, New York, pp. 353-365; Lopez-Berestein, ibid., pp. 3 17-327; see generally ibid.).

In yet another embodiment, the composition can be delivered in a controlled release system. In one embodiment, a pump may be used (Langer, supra; Sefton, 1987, CRC Crit. Ref. Biomed. Eng. 14:20; Buchwald et al., 1980, Surgery 88:507; Saudek et al., 1989, N. Engl. J. Med. 321:574). In another embodiment, polymeric materials can be used (e.g., Medical Applications of Controlled Release, 1974, Langer and Wise (eds.), CRC Pres., Boca Raton, Florida; Controlled Drug Bioavailability, Drug Product Design and Performance, 1984, Smolen and Ball (eds.), Wiley, New York; Ranger and Peppas, 1983, J. Macromol. Sci. Rev. Macromol. Chem. 23:61; Levy et al., 1985, Science 228:190; During et al., 1989,

Ann. Neurol. 25:351; Howard et al., 1989, J.Neurosurg. 7 1:105); U.S. Patent No. 5,679,377; U.S. Patent No. 5,916,597; U.S. Patent No. 5,912,015; U.S. Patent No. 5,989,463; U.S. Patent No. 5,128,326; PCT Publication No. WO 99/15154; and PCT Publication No. WO 99/20253. In yet another embodiment, a controlled release system can be placed in proximity of the therapeutic target, e.g., the urogenital tract, thus requiring only a fraction of the systemic dose (e.g., Goodson, 1984, in Medical Applications of Controlled Release, supra, vol. 2, pp. 115-138).

5

10

15

25

30

35

Other controlled release systems are discussed in the review by Langer (1990, Science 249:1527-1533).

In a specific embodiment where the composition of the invention is a nucleic acid encoding a mutant polypeptide, a mutant polypeptide complex or a fragments thereof, the nucleic acid can be administered *in vivo* to promote expression of its encoded mutant polypeptide compositions, by constructing it as part of an appropriate nucleic acid expression vector and administering it so that it becomes intracellular, *e.g.*, by use of a retroviral vector (U.S. Patent No. 4,980,286), or by direct injection, or by use of microparticle bombardment (*e.g.*, a gene gun; Biolistic, Dupont), or coating with lipids or cell-surface receptors or transfecting agents, or by administering it in linkage to a homeobox-like peptide which is known to enter the nucleus (*e.g.*, Joliot *et al.*, 1991, *Proc. Natl. Acad. Sci. USA* 88:1864-1868), etc. Alternatively, a nucleic acid can be introduced intra-cellularly and incorporated within host cell DNA for expression by homologous recombination.

Accordingly, also provided by the invention is a method for vaccinating a primate against urogenital tract infection, which method comprises administering to the primate a purified nucleic acid containing a nucleotide sequence encoding a mutant peptide or peptide complex comprising a mutant type 1 pilin polypeptide associated with a bacterium that causes a urogenital tract infection, said nucleic acid being administered in an amount effective to produce immunoglobulin molecules that specifically bind the type 1 pilin attachment domain. Pharmaceutical compositions containing nucleic acids comprising nucleotide sequences encoding bacterial adhesin proteins, or fragments or complexes thereof, are also provided.

The dosage of the pharmaceutical formulation can be determined readily by the skilled artisan, for example, by first identifying doses effective to elicit a prophylactic or therapeutic immune response, e.g., by measuring the serum titer of vaccine specific immunoglobulins or by measuring the inhibitory ratio of serum samples, or urine samples, or mucosal secretions. In particular, doses that result in serum endpoint titers of at least

1:800, at least 1:1600, or at least 1:3200 and/or, which have at least 50% binding inhibition of *E. coli* to bladder cells, upon sample dilutions of at least 1:50, at least 1:100, at least 1:200, at least 1:400, at least 1:800, at least 1:1600, or at least 1:3200, and most preferably at least 1:1600, or have detectable specific and, preferably inhibitory immunoglobulins in urine or mucosal secretions, as taught in Section 5.3.3, in an animal model, such as a Cynomolgus monkey, before identifying the optimal dosage in humans.

5

10

15

20

25

30

35

In preferred embodiments, a dose of the purified mutant FimCH complex of 1 μg, 5 μg, 10 μg, 20 μg, 30 μg, 50 μg, 75 μg, 100 μg, 123 μg, 150 μg, or 200 μg, or preferably 25 μg is administered. In other embodiments, the dosage is in the range of 0.25 μg to 1 μg, 1 μg to 5 μg, 1 μg to 10 μg, 1 μg to 20 μg, 1 μg to 50 μg, 1 μg to 75 μg, 1 μg to 100 μg, 1 μg to 150 μg, 1 μg to 200 μg, 5 μg to 10 μg, 10 μg to 15 μg, 10 μg to 20 μg, 15 μg to 25 μg, 20 μg to 30 μg, 30 μg to 50 μg, 25 μg to 75 μg, 50 μg to 100 μg, 75 μg to 125 μg, 50 μg to 125 μg, 50 μg to 200 μg, or 100 μg to 200 μg. For pediatric uses, a fractional dose of the pharmaceutical composition may be administered. For adult patients or patients with persistent infections, larger doses may also be used.

Vaccines of the invention may also be administered on a dosage schedule, for example, an initial administration of the vaccine composition with subsequent booster administrations. In particular embodiments, a second dose of the pharmaceutical composition is administered anywhere from two weeks to one year, preferably from one to six months, after the initial administration. Additionally, a third dose may be administered after the second dose and from three months to two years, or even longer, preferably 4 to 6 months, or 6 months to one year after the initial administration. The third dose may be optionally administered when no or low levels of specific immunoglobulins are detected in the serum and/or urine or mucosal secretions of the subject after the second dose. In a preferred embodiment, a second dose is administered approximately one month after the first administration and a third dose is administered approximately six months after the first administration. In another preferred embodiment, the second dose is administered six months after the first administration.

5.3.3 DETERMINATION OF VACCINE EFFICACY

Immunopotency of the pharmaceutical formulations can be determined by monitoring the immune response of a subject following immunization with a mutant protein composition, in particular the generation of immunoglobulins, particularly IgGs, which are detectable in the urine or mucosal secretions of the subject. Generation of a humoral response may be taken as an indication of a generalized immune response, other components

of which, particularly cell-mediated immunity, may be important for protection against certain disorders. The disorder is UTI in a preferred embodiment. Vaccine efficacy for other mutant proteins for other indications may be determined by analogous methods using skill in the art.

5

10

Subjects can include any primate including Cynomolgus monkeys, chimpanzees and human subjects in well controlled clinical settings. In addition, bacteria causing UTI can be used to induce infection in primates experimentally. However, since many primates are a protected species, the antibody response to a vaccine of the invention can first be studied in a number of smaller, less expensive animals, with the goal of finding one or two best candidate viruses or best combinations of viruses to use in primate efficacy studies. As one example, UTI vaccines of the invention may be tested first in mice for the ability to induce an antibody response to mutant bacterial adhesin polypeptides or polypeptide complexes and to protect against bacterial challenge.

15

The methods of introduction of the vaccine in the test subjects may include oral, intradermal, intramuscular, intravenous, subcutaneous, intranasal or any other standard routes of immunization.

20

The immune response of the test subjects can be analyzed by various approaches such as: the reactivity of the resultant immune serum or urine or mucosal secretions to *E. coli* pilus, as assayed by known techniques, *e.g.*, enzyme linked immunosorbent assay (ELISA), immunoblots, radio-immunoprecipitations, etc.; or protection from UTI infections and/or attenuation of UTI symptoms in immunized hosts, for example, but not limited to, cystitis; or inhibition of binding of *E. coli* to cell surface residues, particularly mannose residues.

25

Urine and mucosa samples may be taken from the test subject every one or two weeks, and serum analyzed for inhibitory antibodies to *E. coli* Type 1 pilus using, *e.g.*, a functional test for inhibitory activity such as measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to transformed human bladder J82 cell line. The presence of antibodies specific for that particular mutant FimH may be assayed by ELISA using the mutant Fim CH for capture protein.

30

Cynomolgus monkeys (*Macaca fascicularis*) may be used to test for immunogenicity of FimH vaccine formulations of the invention. In a specific embodiment, monkeys each receive intramuscularly approximately 100 µg or other appropriate dose of the mutant adhesin in adjuvant. A control Cynomolgus monkey receives adjuvant alone. Blood is drawn weekly for 12 weeks, and serum is analyzed for functionally inhibitory antibodies

35

to the adhesin. Urine and vaginal samples are taken to assess, by ELISA or other antibody detection tests, particularly IgG secretion.

Furthermore, the antibodies that are produced in response to the vaccine can be assessed for functional activity, e.g., binding to the adhesin or inhibiting binding of type 1 pilin bacteria to urogenital tract cells.

5

10

15

20

25

30

35

A non-limiting example of a binding inhibition assay is as follows. Type 1 piliated NU14 *E. coli* are directly labeled with fluorescein isothiocyanate (FITC) and incubated with J82 bladder cells at a ratio of 250 bacteria/cell in the presence of preimmune or immunized serum and incubated for 30 minutes at 37° C. After multiple washes, samples are assayed by flow cytometry, and percent inhibition of bacterial binding to the cells is determined. The samples, such as serum samples, urine samples or vaginal wash samples, are diluted at 1:2, 1:4, 1:8, up to 1:3200 or more, and compared relative to preimmune samples from each subject, in order to identify an endpoint dilution where the binding inhibition is equal to or less than 50%. The binding ratio is defined as the ratio of the number of bacteria or the mean channel fluorescent (MCF) value which correlates with the number of bacteria (*e.g.* NU14) bound to a cell (*e.g.*, J82) in the presence of a diluted sample from an immunized subject, relative to the number of bacteria which bind a cell in the presence of preimmune sample from a non-immunized subject.

Another non-limiting example of a binding inhibition assay is as follows. Briefly, Immulon-4 plates (Dynex Technologies, Inc., Chantilly, VA) are coated with 2.5 µg/ml (100 ml/well) of tri-mannose-BSA (V-Labs, Covington, LA). Type 1-piliated NU14 *E. coli* are added to each well, incubated at 37°C for 1 hour and after extensive washing, bound bacteria are detected with a 1:400 dilution of an anti-*E. coli*-HRP conjugated antibody (Biodesign, Kennebunk, ME). OD₄₀₅ readings of these samples establish the full signal values (FSV) for binding to trimannose (approximately 2.0). Additional samples are run in the presence of 1:50 dilutions of serum to assess inhibition, where percent inhibition equals the FSV - the sample value/FSV x 100. All samples are run in triplicate.

5.4 PHARMACEUTICAL FORMULATIONS AND ADMINISTRATION OF ANTIBODIES

The present invention is directed to antibody-based therapies which involve administering antibodies of the invention or fragments thereof to a mammal, preferably a human, for preventing, treating, or ameliorating symptoms associated with an infection. Prophylactic and therapeutic compounds of the invention include, but are not limited to, antibodies of the invention (including fragments, analogs and derivatives thereof as

described herein) and nucleic acids encoding antibodies of the invention (including fragments, analogs and derivatives thereof and anti-idiotypic antibodies as described herein). Antibodies of the invention or fragments thereof may be provided in pharmaceutically acceptable compositions as known in the art or as described herein.

5

10

Antibodies of the present invention or fragments thereof that function as inhibitors of infection caused by a pathogen can be administered to a mammal, preferably a human, to treat, prevent or ameliorate one or more symptoms associated with infection. For example, antibodies or fragments thereof which disrupt or prevent the interaction between an antigen and its binding partner (e.g., host cell receptor) may be administered to a mammal, preferably a human, to treat, prevent or ameliorate one or more symptoms associated with a infection.

15

It is preferred to use high affinity and/or potent *in vivo* inhibiting antibodies and/or neutralizing antibodies that immunospecifically binds to a the pathogen antigen (e.g., FimH), for prevention of infection and therapy for infection. It is also preferred to use polynucleotides encoding high affinity and/or potent *in vivo* inhibiting antibodies and/or neutralizing antibodies that immunospecifically bind to the pathogen antigen.

In a specific embodiment, an antibody of the present invention or fragment

20

thereof inhibits or decreases the pathogen's ability to infect a host by at least 99%, at least 95%, at least 80%, at least 75%, at least 70%, at least 60%, at least 50%, at least 45%, at least 45%, at least 35%, at least 30%, at least 25%, at least 20%, or at least 10% relative to pathogen infection in absence of said antibodies or antibody fragments. In another embodiment, a combination of antibodies, a combination of antibody fragments, or a combination of antibodies and antibody fragments is used in the methods of the present invention. In a further embodiment, both the vaccines and antibodies can be used in combination to prevent, treat or manage disease or infection.

25

One or more antibodies of the present invention or fragments thereof that immunospecifically bind to one or more pathogen mutant antigens may be used locally or systemically in the body as a therapeutic.

30

35

In one embodiment, a mammal, preferably a human, is administered a first dose of a therapeutic or pharmaceutical composition comprising less than 15 mg/kg, preferably less than 10 mg/kg, less than 5 mg/kg, less than 3 mg/kg, less than 1 mg/kg or less than 0.5 mg/kg of one or more antibodies of the invention or fragments thereof for the prevention of an infection in an amount effective to induce a serum titer of at least 1 μ g/ml, preferably at least 2 μ g/ml, at least 5 μ g/ml, at least 10 μ g/ml, at least 15 μ g/ml, at least 20 μ g/ml, or at least 25 μ g/ml 20 days (preferably 25, 30, 35, 40 days) after the administration

of the first dose and prior to the administration of a subsequent dose. Preferably, the serum titer of said antibodies or antibody fragments is less than 30 μ g/ml 30 days after the administration of the first dose and prior to the administration of a subsequent dose.

The present invention encompasses sustained release formulations comprising one or more antibodies or fragments thereof which have increased *in vivo* half-lives.

5

10

15

20

25

30

35

5.4.1 METHODS OF ADMINISTRATION OF ANTIBODIES

The invention provides methods of treatment, prophylaxis, and amelioration of one or more symptoms associated with pathogen infection by administrating to a subject of an effective amount of antibody or fragment thereof, or pharmaceutical composition comprising an antibody of the invention or fragment thereof. In a preferred aspect, an antibody or fragment thereof is substantially purified (*i.e.*, substantially free from substances that limit its effect or produce undesired side-effects). The subject is preferably a mammal such as non-primate (*e.g.*, cows, pigs, horses, cats, dogs, rats etc.) and a primate (*e.g.*, monkey such as a cynomolgous monkey and a human). In a preferred embodiment, the subject is a human. In specific embodiments, the subject is a woman. The antibodies are particularly useful in women previously infected with UTI, pregnant women and sexually active women. Finally, women previously infected with sexually transmitted diseases or otherwise at risk of UTI are recipients of the antibodies of the invention. In other embodiments, the subject is a diabetic, preferably a diabetic woman. In another embodiment, antibodies to WT FimCH can be administered to a diabetic subject.

Various delivery systems are known and can be used to administer an antibody of the invention or a fragment thereof, e.g., encapsulation in liposomes, microparticles, microcapsules, recombinant cells capable of expressing the antibody or antibody fragment, receptor-mediated endocytosis (see, e.g., Wu and Wu, 1987, J. Biol. Chem. 262:4429-4432), construction of a nucleic acid as part of a retroviral or other vector, etc. Methods of administering an antibody or fragment thereof, or pharmaceutical composition include, but are not limited to, parenteral administration (e.g., intradermal, intramuscular, intraperitoneal, intravenous and subcutaneous), epidural, mucosal (e.g., intranasal, vaginal, buccal and oral routes), oral and topical. In a specific embodiment, antibodies of the present invention or fragments thereof, or pharmaceutical compositions are administered intramuscularly, intravenously, or subcutaneously. The compositions may be administered by any convenient route, for example by infusion or bolus injection, by absorption through epithelial or mucocutaneous linings (e.g., oral mucosa, rectal and

intestinal mucosa, etc.) and may be administered together with other biologically active agents. Administration can be systemic or local. In addition, pulmonary administration can also be employed, *e.g.*, by use of an inhaler or nebulizer, and formulation with an aerosolizing agent. See, *e.g.*, U.S. Patent Nos. 6,019,968, 5,985, 320, 5,985,309, 5,934,272, 5,874,064, 5,855,913, 5,290,540, and 4,880,078, and PCT Publication Nos. WO 92/19244, WO 97/32572, WO 97/44013, WO 98/31346, and WO 99/66903, each of which is incorporated herein by reference their entirety.

5

10

15

20

25

30

35

The invention also provides that an antibody or fragment thereof is packaged in a hermetically sealed container such as an ampoule or sachette indicating the quantity of antibody or antibody fragment. In one embodiment, the antibody or antibody fragment is supplied as a dry sterilized lyophilized powder or water free concentrate in a hermetically sealed container and can be reconstituted, e.g., with water or saline to the appropriate concentration for administration to a subject. Preferably, the antibody or antibody fragment is supplied as a dry sterile lyophilized powder in a hermetically sealed container at a unit dosage of at least 5 mg, more preferably at least 10 mg, at least 15 mg, at least 25 mg, at least 35 mg, at least 45 mg, at least 50 mg, or at least 75 mg. The lyophilized antibody or antibody fragment should be stored at between 2 and 8°C in its original container and the antibody or antibody fragment should be administered within 12 hours, preferably within 6 hours, within 5 hours, within 3 hours, or within 1 hour after being reconstituted. In an alternative embodiment, an antibody or fragment thereof is supplied in liquid form in a hermetically sealed container indicating the quantity and concentration of the antibody or antibody fragment. Preferably, the liquid form of the antibody or fragment thereof is supplied in a hermetically sealed container at least 1 mg/ml, more preferably at least 2.5 mg/ml, at least 5 mg/ml, at least 8 mg/ml, at least 10 mg/ml, at least 15 mg/kg, or at least 25 mg/ml.

In a specific embodiment, it may be desirable to administer the pharmaceutical compositions of the invention locally to the area in need of treatment; this may be achieved by, for example, and not by way of limitation, local topical administration, local infusion, by injection, or by means of an implant, said implant being of a porous, non-porous, or gelatinous material, including membranes, such as sialastic membranes, or fibers. Preferably, when administering a an antibody of the invention or fragment thereof, care must be taken to use materials to which the antibody or antibody fragment does not absorb.

In another embodiment, the composition can be delivered in a vesicle, in particular a liposome (see Langer, 1990, Science 249:1527-1533; Treat *et al.*, 1989, in

PCT/US01/47994 WO 02/102974

Liposomes in the Therapy of Infectious Disease and Cancer, Lopez-Berestein and Fidler (eds.), Liss, New York, pp. 353-365; Lopez-Berestein, ibid., pp. 317-327; see generally ibid.).

5

20

25

30

35

In yet another embodiment, the composition can be delivered in a controlled release system. In one embodiment, a pump may be used (see Langer, supra; Sefton, 1987, CRC Crit. Ref. Biomed. Eng. 14:20; Buchwald et al., 1980, Surgery 88:507; Saudek et al., 1989, N. Engl. J. Med. 321:574). In another embodiment, polymeric materials can be used to achieve controlled release of the antibodies of the invention or fragments thereof (see e.g., Medical Applications of Controlled Release, Langer and Wise (eds.), CRC Pres., Boca 10 Raton, Florida (1974); Controlled Drug Bioavailability, Drug Product Design and Performance, Smolen and Ball (eds.), Wiley, New York (1984); Ranger and Peppas, 1983, J., Macromol. Sci. Rev. Macromol. Chem. 23:61; see also Levy et al., 1985, Science 228:190; During et al., 1989, Ann. Neurol. 25:351; Howard et al., 1989, J. Neurosurg. 7 1:105); U.S. Patent No. 5,679,377; U.S. Patent No. 5,916,597; U.S. Patent No. 5,912,015; 15 U.S. Patent No. 5,989,463; U.S. Patent No. 5,128,326; PCT Publication No. WO 99/15154; and PCT Publication No. WO 99/20253. In yet another embodiment, a controlled release system can be placed in proximity of the therapeutic target, i.e., the lungs, thus requiring only a fraction of the systemic dose (see, e.g., Goodson, in Medical Applications of Controlled Release, supra, vol. 2, pp. 115-138 (1984)).

Other controlled release systems are discussed in the review by Langer (1990, Science 249:1527-1533).

In yet another embodiment, compositions comprising antibodies of the invention or fragments thereof are formulated for sustained release. Any technique known to one of skill in the art can be used to produce sustained release formulations comprising one or more antibodies of the invention or fragments thereof. See, e.g., U.S. Patent No. 4,526,938, PCT publication WO 91/05548, PCT publication WO 96/20698, Ning et al., 1996, "Intratumoral Radioimmunotheraphy of a Human Colon Cancer Xenograft Using a Sustained-Release Gel," Radiotherapy & Oncology 39:179-189, Song et al., 1995, "Antibody Mediated Lung Targeting of Long-Circulating Emulsions," PDA Journal of Pharmaceutical Science & Technology 50:372-397, Cleek et al., 1997, "Biodegradable Polymeric Carriers for a bFGF Antibody for Cardiovascular Application," Pro. Int'l. Symp. Control. Rel. Bioact. Mater. 24:853-854, and Lam et al., 1997, "Microencapsulation of Recombinant Humanized Monoclonal Antibody for Local Delivery," Proc. Int'l. Symp. Control Rel. Bioact. Mater. 24:759-760, each of which is incorporated herein by reference in their entirety.

In a specific embodiment where the composition of the invention is a nucleic acid encoding an antibody or antibody fragment, the nucleic acid can be administered *in vivo* to promote expression of its encoded antibody or antibody fragment, by constructing it as part of an appropriate nucleic acid expression vector and administering it so that it becomes intracellular, *e.g.*, by use of a retroviral vector (see U.S. Patent No. 4,980,286), or by direct injection, or by use of microparticle bombardment (*e.g.*, a gene gun; Biolistic, Dupont), or coating with lipids or cell-surface receptors or transfecting agents, or by administering it in linkage to a homeobox-like peptide which is known to enter the nucleus (*see e.g.*, Joliot *et al.*, 1991, *Proc. Natl. Acad. Sci.* USA 88:1864-1868), etc. Alternatively, a nucleic acid can be introduced intracellularly and incorporated within host cell DNA for expression by homologous recombination.

5

15

20

25

30

35

The present invention also provides pharmaceutical compositions. Such compositions comprise a prophylactically or therapeutically effective amount of an antibody or a fragment thereof, and a pharmaceutically acceptable carrier. In a specific embodiment, the term "pharmaceutically acceptable" means approved by a regulatory agency of the Federal or a state government or listed in the U.S. Pharmacopeia or other generally recognized pharmacopeia for use in animals, and more particularly in humans. The term "carrier" refers to a diluent, adjuvant (e.g., Freund's adjuvant (complete and incomplete)), excipient, or vehicle with which the therapeutic is administered. Such pharmaceutical carriers can be sterile liquids, such as water and oils, including those of petroleum, animal, vegetable or synthetic origin, such as peanut oil, soybean oil, mineral oil, sesame oil and the like. Water is a preferred carrier when the pharmaceutical composition is administered intravenously. Saline solutions and aqueous dextrose and glycerol solutions can also be employed as liquid carriers, particularly for injectable solutions. Suitable pharmaceutical excipients include starch, glucose, lactose, sucrose, gelatin, malt, rice, flour, chalk, silica gel, sodium stearate, glycerol monostearate, talc, sodium chloride, dried skim milk, glycerol, propylene, glycol, water, ethanol and the like. The composition, if desired, can also contain minor amounts of wetting or emulsifying agents, or pH buffering agents. These compositions can take the form of solutions, suspensions, emulsion, tablets, pills, capsules, powders, sustained-release formulations and the like. Oral formulation can include standard carriers such as pharmaceutical grades of mannitol, lactose, starch, magnesium stearate, sodium saccharine, cellulose, magnesium carbonate, etc. Examples of suitable pharmaceutical carriers are described in "Remington's Pharmaceutical Sciences" by E.W. Martin. Such compositions will contain a prophylactically or therapeutically effective amount of the antibody or fragment thereof, preferably in purified form, together with a

suitable amount of carrier so as to provide the form for proper administration to the patient. The formulation should suit the mode of administration.

In a preferred embodiment, the composition is formulated in accordance with routine procedures as a pharmaceutical composition adapted for intravenous administration to human beings. Typically, compositions for intravenous administration are solutions in sterile isotonic aqueous buffer. Where necessary, the composition may also include a solubilizing agent and a local anesthetic such as lignocamne to ease pain at the site of the injection.

5

20

35

Generally, the ingredients of compositions of the invention are supplied

either separately or mixed together in unit dosage form, for example, as a dry lyophilized powder or water free concentrate in a hermetically sealed container such as an ampoule or sachette indicating the quantity of active agent. Where the composition is to be administered by infusion, it can be dispensed with an infusion bottle containing sterile pharmaceutical grade water or saline. Where the composition is administered by injection, an ampoule of sterile water for injection or saline can be provided so that the ingredients may be mixed prior to administration.

The compositions of the invention can be formulated as neutral or salt forms. Pharmaceutically acceptable salts include those formed with anions such as those derived from hydrochloric, phosphoric, acetic, oxalic, tartaric acids, etc., and those formed with cations such as those derived from sodium, potassium, ammonium, calcium, ferric hydroxides, isopropylamine, triethylamine, 2-ethylamino ethanol, histidine, procaine, etc.

5.5 RECOMBINANT NUCLEIC ACIDS

Nucleic acid sequences changes can be introduced by mutation thereby
leading to changes in the amino acid sequence of the encoded protein. For example, one can make nucleotide substitutions leading to amino acid substitutions at "non-essential" amino acid residues. A "non-essential" amino acid residue is a residue that can be altered from the wild-type sequence without altering the biological activity, whereas an "essential" amino acid residue is required for biological activity. For example, amino acid residues that are not conserved or only semi-conserved among homologous of various species may be non-essential for activity and thus would be likely targets for alteration. Alternatively, amino acid residues that are conserved among the homologous of various species (e.g., murine and human) may be essential for activity and thus would not be likely targets for alteration.

Accordingly, another aspect of the invention pertains to nucleic acid molecules encoding a polypeptide of the invention that contain changes in amino acid

residues. Such polypeptides differ in amino acid sequence from wild type protein. In one embodiment, the domain which interacts with the wild type protein's binding partner is mutated. For example, in the bacterial adhesin FimH, amino acid substitutions can be introduced into residues listed in Section 5.1 above.

5

An isolated nucleic acid molecule encoding a variant protein can be created by introducing one or more nucleotide substitutions, additions or deletions into the nucleotide sequence, such that one or more amino acid substitutions, additions or deletions are introduced into the encoded protein. Mutations can be introduced by standard techniques, such as site-directed mutagenesis and PCR-mediated mutagenesis. Briefly, PCR primers are designed that delete the trinucleotide codon of the amino acid to be changed and replace it with the trinucleotide codon of the amino acid to be included. This primer is used in the PCR amplification of DNA encoding the protein of interest. This fragment is then isolated and inserted into the full length cDNA encoding the protein of interest and expressed recombinantly. The resulting protein now includes the amino acid replacement.

15

20

10

Preferably, non-conservative amino acid substitutions are made at one or more amino acid residues. Non-conservative replacements are those that take place between families of amino acids that are unrelated in their side chains. Genetically encoded amino acids are can be divided into four families: (1) acidic = aspartate, glutamate; (2) basic = lysine, arginine, histidine; (3) nonpolar = alanine, valine, leucine, isoleucine, proline, phenylalanine, methionine, tryptophan; and (4) uncharged polar = glycine, asparagine, glutamine, cysteine, serine, threonine, tyrosine. In similar fashion, the amino acid repertoire can be grouped as (1) acidic = aspartate, glutamate; (2) basic = lysine, arginine histidine, (3) aliphatic = glycine, alanine, valine, leucine, isoleucine, serine, threonine, with serine and threonine optionally be grouped separately as aliphatic-hydroxyl; (4) aromatic = phenylalanine, tyrosine, tryptophan; (5) amide = asparagine, glutamine; and (6) sulfur - containing = cysteine and methionine. (See, for example, Biochemistry, 4th ed., Ed. by L. Stryer, WH Freeman and Co.: 1995).

25

Alternatively, mutations can be introduced randomly along all or part of the coding sequence, such as by saturation mutagenesis.

30

35

Mutagenesis may be performed in accordance with any of the techniques known in the art including, but not limited to, synthesizing an oligonucleotide having one or more modifications within the sequence to be modified. Site-specific mutagenesis allows the production of mutants through the use of specific oligonucleotide sequences which encode the DNA sequence of the desired mutation, as well as a sufficient number of adjacent nucleotides, to provide a primer sequence of sufficient size and sequence complexity to form

a stable duplex on both sides of the deletion junction being traversed. Typically, a primer of about 17 to about 75 nucleotides or more in length is preferred, with about 10 to about 25 or more residues on both sides of the junction of the sequence being altered. A number of such primers introducing a variety of different mutations at one or more positions may be used to generated a library of mutants.

The technique of site-specific mutagenesis is well known in the art, as exemplified by various publications (see, e.g., Kunkel et al., Methods Enzymol., 154:367-82, 1987, which is hereby incorporated by reference in its entirety). In general, site-directed mutagenesis is performed by first obtaining a single-stranded vector or melting apart of two strands of a double stranded vector which includes within its sequence a DNA sequence which encodes the desired peptide. An oligonucleotide primer bearing the desired mutated sequence is prepared, generally synthetically. This primer is then annealed with the single-stranded vector, and subjected to DNA polymerizing enzymes such as T7 DNA polymerase, in order to complete the synthesis of the mutation-bearing strand. Thus, a heteroduplex is formed wherein one strand encodes the original non-mutated sequence and the second strand bears the desired mutation. This heteroduplex vector is then used to transform or transfect appropriate cells, such as E. coli cells, and clones are selected which include recombinant vectors bearing the mutated sequence arrangement. As will be appreciated, the technique typically employs a phage vector which exists in both a single stranded and double stranded form. Typical vectors useful in site-directed mutagenesis include vectors such as the M13 phage. These phage are readily commercially available and their use is generally well known to those skilled in the art. Double stranded plasmids are also routinely employed in site directed mutagenesis which eliminates the step of transferring the gene of interest from a plasmid to a phage.

Alternatively, the use of PCRTM with commercially available thermostable enzymes such as *Taq* DNA polymerase may be used to incorporate a mutagenic oligonucleotide primer into an amplified DNA fragment that can then be cloned into an appropriate cloning or expression vector. See, *e.g.*, Tomic *et al.*, 1987, *Nucleic Acids Res.*, 18:1656; Upender *et al.*, 1995, *BioTechniques*, 18:29-30, 32, 1995, for PCRTM -mediated mutagenesis procedures, which are hereby incorporated in their entireties. PCRTM employing a thermostable ligase in addition to a thermostable polymerase may also be used to incorporate a phosphorylated mutagenic oligonucleotide into an amplified DNA fragment that may then be cloned into an appropriate cloning or expression vector (see *e.g.*, Michael, 1994, *BioTechniques*, 16:410-2, which is hereby incorporated by reference in its entirety).

35

30

5

10

15

20

25

Following mutagenesis, the encoded protein can be expressed recombinantly and the activity of the protein can be determined. Those showing desired activity can then be further characterized. In the present invention, mutant proteins which lose or have decreased biological activity (e.g., binding) are of particular interest.

5

10

15

20

25

30

35

5.6 PROTEIN EXPRESSION AND PURIFICATION

The mutant adhesin proteins, complexes and fragments thereof (preferably mutant FimH proteins and polypeptides) maybe produced by any method available in the art. Those skilled in the art will readily be able to purify such proteins, fragments or complexes by routine techniques.

One problem with utilizing such proteins has been that synthesis of the polypeptide, such as FimH, results in a protein that falls short of attaining its native in vivo structure. Thus, there is a difference between the in vivo conformation of such a protein and that attained by a purified recombinant form of such protein. The reason for this difference in conformation has been determined. In general, a pilin protein, such as an adhesin like FimH, has a native conformation that is at least partly determined by the in vivo interaction of such protein with an additional protein, here a periplasmic chaperone protein called FimC. The resulting FimC-FimH (or FimCH) complex is the form that presents the native FimH conformation as seen in vivo and thus by the immune system (Choudhury et al., 1999, Science 285, 1061; Sauer et al., 1999, Science 285:1058). Consequently, the methods and compositions of the invention include such complexes where said proteins are co-expressed, or otherwise formed in a combined state, with their respective periplasmic chaperone thereby yielding the native complex normally seen in vivo by the immune system following infection by a disease causing pathogen. Accordingly, the present invention further encompasses administration of such pilin complexes, i.e., complexes of FimC with a FimH polypeptide.

FimH complexes can be readily produced by recombinant methods in such a way as to incorporate therein the sequences provided by FimC in the FimCH complex, thus yielding a native structure for FimH, which structure is immunogenic in nature. In essence, the portion of the FimC molecule that binds to FimH and directs its native conformation is engineered into the FimH structure itself, at the appropriate location, to result in a native FimH structure. This portion of the FimC molecule that binds to FimH in the FimCH complex is called a "donor strand" and the mechanism of formation of the native FimH structure using only this additional strand from FimC has been referred to as "donor strand complementation." Thus, the FimH complexes, can be produced in their "donor

complemented" form to provide highly immunogenic structures for use in therapeutically effective vaccine compositions within the present invention. Such donor strand complemented forms are disclosed in detail in U.S. Application No. 09/615,846, filed July 13, 2000 and PCT/US00/19066, filed July 13, 2000, both entitled "Donor Strand Complemented Pilus-Based Vaccines", each of which is hereby incorporated by reference herein in its entirety.

Accordingly, in preferred embodiments, complexes of FimH and FimC are administered in the methods of the invention. Such complexes include FimH-FimC fusion proteins and complexes, preferably, containing an equimolar ratio of FimH and FimC. Any known FimC protein can be used in such complexes. Preferably the FimC protein is from the *E. coli* J96 isolate and has an amino acid sequence of Figure 1. In a more preferred embodiment, a FimCH complex containing a FimH protein and a FimC protein in equimolar amounts is administered, preferably where the FimH protein has an amino acid sequence (with one or more amino acid modifications, as discussed above) of Figure 1 and the FimC protein has an amino acid sequence of Figure 1. As described *infra*, the FimCH complexes can be expressed from the same plasmid, preferably under the control of separate promoters, and isolated from the host cell, *e.g.*, an *E. coli* host cell.

Complexes comprising the *E. coli* chaperone FimC and a FimH variant of the invention may be formed by co-expressing a FimH variant polypeptide, whose amino acid and nucleotide sequences are known in the art (such as the FimH having the amino acid sequence of Figure 1) along with a FimC variant polypeptide, whose amino acid and nucleotide sequences are known in the art (such as the FimC having the amino acid sequence of Figure 1), from a recombinant cell.

In addition, the FimC-mutant FimH complexes useful in vaccines can be recovered from the periplasmic spaces of cells of the indicated strains disclosed herein. These complexes are found in relatively large amounts in recombinant *E. coli* strains which express the FimC protein at levels in excess of those produced in wild type strains. A suitable recombinant strain is C600/pHJ9205, in which expression of FimC has been put under control of the arabinose promoter. Those skilled in the art will recognize that other promoter sequences that can be regulated easily may also be used. Of course, such cells are readily engineered to express one or more of the FimH variant polypeptides of the invention. An extract of periplasm is obtained by exposing the bacteria to lysozyme in the presence of a hypertonic sucrose solution. FimCH complexes can also be purified using conventional protein purification methods well known in the art.

30

5

10

15

20

25

In a similar manner, FimH fragments can be recombinantly produced either by having *E. coli* produce the full-length FimH and then fragmenting the protein or may be isolated by mannose-binding affinity purification. Thus, only fragments of the FimH protein that retain mannose binding are isolated. Preferably, such mannose-binding fragments have a label such as a his-tag included and may be purified by methods such as nickel chromatography.

5

10

15

20

25

30

35

In accordance with the foregoing, FimC of *E. coli* is available through the American Type Culture Collection (ATCC) as accession number Z37500. A FimH protein of *E. coli* is available as ATCC Accession No. 1361011.

The polynucleotides encoding the mutant protein or polypeptide above may have the coding sequence fused in frame to a marker sequence which allows for purification of the polypeptides of the present invention. The marker sequence may be, for example, a hexa-histidine tag supplied by a pQE-9 vector to provide for purification of the mature polypeptides fused to the marker in the case of a bacterial host, or, for example, the marker sequence may be a hemagglutinin (HA) tag when a mammalian host, e.g. COS-7 cells, is used. The HA tag corresponds to an epitope derived from the influenza hemagglutinin protein (Wilson, et al., 1984, Cell, 37:767).

The proteins and polypeptide of the invention may be recombinantly produced in an *E. coli* species host. Mutant FimH may likewise be produced recombinantly by producing the appropriate donor strand complemented version of FimH, wherein the amino acid sequence of FimC that interacts with mutant FimH in the FimCH complex is itself engineered at the C-terminal end of mutant FimH to provide the native conformation without the need for the remainder of the FimC molecule to be present. Additionally, mutant FimH variants may also be utilized in the form of a complex comprising isolated domains thereof, especially mannose-binding domains and fragments, which domains or fragments may be linked together, either covalently or non-covalently, utilizing linking segments, such linking segments being formed of amino acid sequences or other oligomeric structures, including simple polymer structures, to provide an overall structure exhibiting immunogenic activity.

In producing said proteins, particularly the adhesin protein recombinantly, a preferred host is a species of bacteria that can be cultured under conditions such that the usher gene (if present) is not expressed. Further preferred is a host species that is missing the usher gene or has a defective usher gene. Even further preferred is a host which is missing the pilus proteins other than the FimH protein (and may also produce the chaperone, such as FimC). When an adhesin protein or a mannose binding fragment of such adhesin

protein is to be produced in the absence of its chaperone protein (or to be separated from the chaperone after production), the mutant adhesin protein (or fragment) may be permitted to become properly folded in the presence of its chaperone protein and is then separated from the chaperone protein.

The present invention also relates to vectors which include polynucleotides encoding one or more of the mutant protein or polypeptides of the present invention, host cells which are genetically engineered with vectors of the invention, including host cells containing a nucleotide sequence encoding a protein of the invention operably linked to a heterologous promoter, and the production of such mutant adhesin proteins and/or chaperone proteins by recombinant techniques in an isolated and substantially immunogenically pure form.

5

10

15

20

25

30

35

Host cells are genetically engineered (transduced or transformed or transfected) with the vectors comprising a polynucleotide encoding a chaperone, mutant adhesin protein, or the like, which may be, for example, a cloning vector or an expression vector. The vector may be, for example, in the form of a plasmid, a viral particle, a phage, etc. The engineered host cells can be cultured in conventional nutrient media modified as appropriate for activating promoters, selecting transformants or amplifying the polynucleotides which encode such polypeptides. The culture conditions, such as temperature, pH and the like, are those previously used with the host cell selected for expression, and will be apparent to the ordinarily skilled artisan.

Vectors include chromosomal, nonchromosomal and synthetic DNA sequences, e.g., derivatives of SV40; bacterial plasmids; phage DNA; baculovirus; yeast plasmids; vectors derived from combinations of plasmids and phage DNA, viral DNA such as retrovirus, vaccinia, adenovirus, fowl pox virus, and pseudorabies. However, any other vector may be used as long as it is replicable and viable in the host.

The appropriate DNA sequence may be inserted into the vector by a variety of procedures. In general, the DNA sequence is inserted into an appropriate restriction endonuclease site(s) by procedures known in the art. Such procedures and others are deemed to be within the scope of those skilled in the art.

The DNA sequence in the expression vector is operatively linked to an appropriate expression control sequence(s) (promoter) to direct mRNA synthesis. As representative examples of such promoters, there may be mentioned: LTR or SV40 promoter, the *E. coli. lac* or *trp*, the phage lambda P_L promoter and other promoters known to control expression of genes in prokaryotic or eukaryotic cells or their viruses. The expression vector also contains a ribosome binding site for translation initiation and a

transcription terminator. The vector may also include appropriate sequences for amplifying expression.

In addition, the expression vectors preferably contain one or more selectable marker genes to provide a phenotypic trait for selection of transformed host cells such as dihydrofolate reductase or neomycin resistance for eukaryotic cell culture, or such as tetracycline or ampicillin resistance in prokaryotic cell culture, e.g., E. coli.

5

10

15

20

25

30

35

Optimal expression of a wild type FimCH complex has been achieved using a newly constructed single vector containing the FimH and FimC genes but having the advantage that each gene is under its own separate lac promoter. Thus, one lac promoter is 5' with respect to FimC while the second lac promoter is 5' to the FimH gene. This plasmid was successfully constructed using the common plasmid pUC19 as a background vector (Yannish-Perron, et al., 1985, Gene, 33:103-119). This new plasmid, when used to transform the host E. coli strain BL21 (as described in Phillips, et al., 1984, J. Bacteriol. 159:283-287) and then induced using IPTG at the mid-logarithmic stage of growth, gives maximal expression of the FimCH complex in the bacterial periplasmic space. This material is then extracted and purified by methods well known in the art, including those described herein. Such a plasmid can be constructed that encodes a wild type FimC in combination with a mutant FimH.

The vector containing the appropriate DNA sequence as hereinabove described, as well as an appropriate promoter or control sequence, may be employed to transform an appropriate host to permit the host to express the proteins.

As representative examples of appropriate hosts, there may be mentioned: bacterial cells, such as *E. coli*, *Streptomyces*, *Salmonella typhimurium*; fungal cells, such as yeast; insect cells such as Drosophila S2 and Spodoptera Sf9; animal cells such as CHO, COS or Bowes melanoma; adenoviruses; plant cells, etc. The selection of an appropriate host is deemed to be within the scope of those skilled in the art from the teachings herein.

Constructs for production of the adhesin proteins comprise a vector, such as a plasmid or viral vector, into which a sequence of the invention has been inserted, in a forward or reverse orientation: The construct may further comprise regulatory sequences, including, for example, a promoter, operably linked to the sequence. Large numbers of suitable vectors and promoters are known to those of skill in the art, and are commercially available. The following vectors are provided by way of example. Bacterial: pQE70, pQE60, pQE-9 (Qiagen, Inc.), pbs, pD10, phagescript, psiX174, pbluescript SK, pbsks, pNH8A, pNH16a, pNH18A, pNH46A (Stratagene); ptrc99a, pKK223-3, pKK233-3, pDR540, pRIT5 (Pharmacia). Eukaryotic: pWLNEO, pSV2CAT, pOG44, pXT1, pSG

(Stratagene) pSVK3, pBPV, pMSG, pSVL (Pharmacia). However, any other plasmid or vector may be used as long as they are replicable and viable in the host.

Promoter regions can be selected from any desired gene using CAT (chloramphenical transferase) vectors or other vectors with selectable markers. Two appropriate vectors are pKK232-8 and pCM7. Particular named bacterial promoters include lacI, lacZ, T3, T7, gpt, lambda P_R , P_L and TRP. Eukaryotic promoters include CMV immediate early, HSV thymidine kinase, early and late SV40, LTRs from retrovirus, and mouse metallothionein-I. Selection of the appropriate vector and promoter is well within the level of ordinary skill in the art.

The host cell for recombinant production can be a higher eukaryotic cell, such as a mammalian cell, or a lower eukaryotic cell, such as a yeast cell, or the host cell can be a prokaryotic cell, such as a bacterial cell. Introduction of the construct into the host cell can be effected by calcium phosphate transfection, DEAE-Dextran mediated transfection, or electroporation (Davis, L., Dibner, M., Battey, I., Basic Methods in Molecular Biology, (1986)).

The constructs in host cells can be used in a conventional manner to produce the gene product encoded by the recombinant sequence. Alternatively, the polypeptides of the invention can be synthetically produced by conventional peptide synthesizers.

Mature proteins can be expressed in mammalian cells, yeast, bacteria, or other cells under the control of appropriate promoters. Cell-free translation systems can also be employed to produce such proteins using RNAs derived from the DNA constructs of the present invention. Appropriate cloning and expression vectors for use with prokaryotic and eukaryotic hosts, as well as other methods in molecular biology, are described in Sambrook, et al., 1989, Molecular Cloning: A Laboratory Manual, Second Edition, Cold Spring Harbor, N.Y.; Wu et al., Methods in Gene Biotechnology (CRC Press, New York, NY, 1997), and Recombinant Gene Expression Protocols, in Methods in Molecular Biology, Vol. 62, (Tuan, ed., Humana Press, Totowa, NJ, 1997), the disclosures of which are hereby incorporated by reference.

Transcription of the DNA encoding the polypeptides of the present invention by higher eukaryotes is increased by inserting an enhancer sequence into the vector. Enhancers are cis-acting elements of DNA, usually about from 10 to 300 bp that act on a promoter to increase its transcription. Examples include the SV40 enhancer on the late side of the replication origin bp 100 to 270, a cytomegalovirus early promoter enhancer, the polyoma enhancer on the late side of the replication origin, and adenovirus enhancers.

30

5

10

15

20

25

Generally, recombinant expression vectors will include origins of replication and selectable markers permitting transformation of the host cell, e.g., the ampicillin resistance gene of E. coli and S. cerevisiae TRP1 gene, and a promoter derived from a highly-expressed gene to direct transcription of a downstream structural sequence. Such promoters can be derived from operons encoding glycolytic enzymes such as 3-phosphoglycerate kinase (PGK), a-factor, acid phosphatase, or heat shock proteins, among others. The heterologous structural sequence is assembled in appropriate phase with translation initiation and termination sequences. Optionally, the heterologous sequence can encode a fusion protein including an N-terminal identification peptide imparting desired characteristics, e.g., stabilization or simplified purification of expressed recombinant product.

5

10

15

20

25

30

35

Useful expression vectors for bacterial use are constructed by inserting a structural DNA sequence encoding a desired protein together with suitable translation initiation and termination signals in operable reading phase with a functional promoter. The vector will comprise one or more phenotypic selectable markers and an origin of replication to ensure maintenance of the vector and to, if desirable, provide amplification within the host. Suitable prokaryotic hosts for transformation include *E. coli, Bacillus subtilis, Salmonella typhimurium* and various species within the genera Pseudomonas, Streptomyces, and Staphylococcus, although others may also be employed as a matter of choice.

As a representative but non-limiting example, useful expression vectors for bacterial use can comprise a selectable marker and bacterial origin of replication derived from commercially available plasmids comprising genetic elements of the well known cloning vector pBR322 (ATCC 37017). Such commercial vectors include, for example, pKK223-3 (Pharmacia Fine Chemicals, Uppsala, Sweden) and GEM1 (Promega Biotec, Madison, WI, USA). These pBR322 "backbone" sections are combined with an appropriate promoter and the structural sequence to be expressed.

Following transformation of a suitable host strain and growth of the host strain to an appropriate cell density, the selected promoter is induced by appropriate means (e.g., temperature shift or chemical induction) and cells are cultured for an additional period.

Cells are typically harvested by centrifugation, disrupted by physical or chemical means, and the resulting crude extract retained for further purification.

Microbial cells employed in expression of proteins can be disrupted by any convenient method, including freeze-thaw cycling, sonication, a french press, mechanical disruption, or use of cell lysing agents, such methods are well know to those skilled in the art.

Various mammalian cell culture systems can also be employed to express recombinant protein. Examples of mammalian expression systems include the COS-7 lines of monkey kidney fibroblasts (described by Gluzman, 1981, Cell, 23:175) and other cell lines capable of expressing a compatible vector, for example, the C127, 3T3, CHO, HeLa and BHK cell lines. Mammalian expression vectors will comprise an origin of replication, a suitable promoter and enhancer, and also any necessary ribosome binding sites, polyadenylation site, splice donor and acceptor sites, transcriptional termination sequences, and 5' flanking nontranscribed sequences. DNA sequences derived from the SV40 splice, and polyadenylation sites may be used to provide the required nontranscribed genetic elements.

The proteins and polypeptides can be recovered and/or purified from recombinant cell cultures by well-known protein recovery and purification methods. Such methodology may include ammonium sulfate or ethanol precipitation, acid extraction, anion or cation exchange chromatography, phosphocellulose chromatography, hydrophobic interaction chromatography, affinity chromatography, hydroxylapatite chromatography and lectin chromatography. Protein refolding steps can be used, as necessary, in completing configuration of the mature protein. In this respect, chaperones may be used in such a refolding procedure. Finally, high performance liquid chromatography (HPLC) can be employed for final purification steps.

20

25

30

35

15

5

10

The polypeptides that are useful as immunogens in the present invention may be a naturally purified product (if a suitable naturally occurring mutant exists), or a product of chemical synthetic procedures, or produced by recombinant techniques from a prokaryotic or eukaryotic host (for example, by bacterial, yeast, higher plant, insect and mammalian cells in culture). Depending upon the host employed in a recombinant production procedure, the polypeptides of the present invention may be glycosylated or may be non-glycosylated. Particularly preferred immunogens are FimH adhesin protein or fragments thereof since FimH is highly conserved among many bacterial species (see Figure 3). Therefore, antibodies against FimH (or its mannose-binding fragments) should bind to FimH of other bacterial species (in addition to E. coli) and vaccines against E. coli FimH (or FimH mannose-binding fragments) should give protection against other bacterial infections in addition to E. coli infections (for example, against other Enterobacteriacea infections) (see, e.g., U.S. Application Serial No. 09/615,846 and PCT application No. PCT/US00/19066, both entitled "Donor Strand Complemented Pilus-Based Vaccines" and filed July 13, 2000; U.S. Application No.09/616,702, filed July 14, 2000, entitled "FimH Adhesin Based Vaccines" by Hultgren et al.; and U.S. Provisional Application No. 60/216,750, filed July 7,

2000, entitled "FimH Adhesin Proteins" by Langermann et al.)

Procedures for the isolation of a periplasmic chaperone protein complexed with an adhesin protein are known in the art, as an example see Jones *et al.*, (1993, *Proc. Natl. Acad. Sci. USA* 90:8397-8401). Further, the individually expressed adhesin proteins may be isolated by recombinant expression/isolation methods that are well-known in the art. Typical examples for such isolation may utilize an antibody to the protein or to a His tag or cleavable leader or tail that is expressing as part of the protein structure.

The FimCH polypeptides useful in forming the vaccine compositions of the present invention may conveniently be cloned using various cloning systems. The FimCH complex described therein is composed of a 52 kDa complex composed of two proteins: FimC (22.8 kDa) and FimH (29.1 kDa) in a 1:1 equimolar ratio. The FimCH complex is expressed from a pUC-based vector (pGCA139-1-1) with two separate lac-inducible promoters driving expression of the FimC and FimH genes, respectively. The FimC and the FimH genes in the pGCA139-1-1 vector were derived from uropathogenic *E. coli* isolate J96 and have the nucleotide sequences of Figure 1.

The FimCH complex is produced in the periplasm of *E. coli* strain BL21 and is purified from periplasmic extracts by standard chromatographic methods. The FimCH protein has been formulated in a number of different buffers compatible with its solubility profile including 20 mM HEPES (pH 7.0), PBS (pH 7.0) and sodium citrate (pH 6.0) in 0.2 M NaCl. This sodium citrate/sodium chloride formulation enhances the stability of the FimCH complex and is also compatible with commonly used diluents.

Plasmid pCGA139-1-1 was constructed as a means of producing relatively large amounts of *E. coli* chaperone-adhesin complex, wild type FimCH. For use in the vaccine compositions disclosed herein, the wild type FimH is replaced with a mutant FimH.

The plasmid vector, pCGA139-1-1, contains the following genetic elements: (1) an *E. coli* FimC chaperone gene followed by (2) the FimH adhesin gene, both from *E. coli* strain J96 (a urinary tract infection (UTI) isolate) each preceded by its respective native signal sequence (nss); (3) a kanamycin resistance (kan' or k') marker; (4) lacl^q which codes for a repressor protein that binds the lac promoter unless it is induced; (5) an inactivated beta-lactamase (bla) gene; (6) pUC origin of replication (ori); and (7) two lac promoters, one preceding the FimC signal and the other preceding that of FimH.

5

10

15

20

25

5.6.1 FUSION PROTEINS

In certain embodiments, the invention provides a polypeptide which is constructed as a fusion protein (e.g., covalently bonded to a different protein). The invention provides nucleic acids encoding such fusion proteins. In certain other embodiments of this invention, the nucleic acid encoding a fusion protein of the invention is operably linked to an appropriate promoter.

Fusion proteins in which a mutant FimH protein, preferably an adhesion or FimH, or a fragment of such a protein is fused to a heterologous protein are within the scope of this invention. In addition, fusion proteins can be made with antibodies of the invention or fragments thereof. Such proteins and peptides can be designed, for example, on the basis of the nucleotide sequences disclosed herein and/or on the basis of the amino acid sequences disclosed herein. Fusion proteins include, but are not limited to fusions to any amino acid sequence that allows the fusion protein to be anchored to the cell membrane; or fusions of the peptide to an enzyme, fluorescent protein, luminescent protein, or a flag epitope protein or peptide which provides a marker function.

In a specific embodiment, a polypeptide of the invention (or a nucleic acid encoding the polypeptide of the invention) is constructed as a chimeric or fusion protein. The polypeptide of the invention is joined at its amino- or carboxy-terminus via a peptide bond to an amino acid sequence of a different protein. In specific embodiments, the amino acid sequence of the different protein is at least 6, 10, 20 or 30 continuous amino acids of the different proteins or a portion of the heterologous protein that is functionally active. In specific embodiments, the amino acid sequence of the different protein is at least 50, 75, 100, or 150 continuous amino acids of the different proteins or a portion of the different protein that is functionally active. In one embodiment, such a chimeric protein is produced by recombinant expression of a nucleic acid encoding a polypeptide of the invention joined in-frame to a coding sequence for a different protein (e.g., such as a heparin binding domain). Such a chimeric product can be made by ligating the appropriate nucleic acid sequences encoding the desired amino acid sequences to each other by methods known in the art, in the proper coding frame, and expressing the chimeric product into the expression vehicle of choice by methods commonly known in the art.

Chimeric nucleic acids comprising portions of a nucleic acid encoding a polypeptide of the invention fused to any heterologous protein-encoding sequences may be constructed. In a specific embodiment, the fusion protein comprises an affinity tag such as a hexahistidine tag, or other affinity tag that may be used in purification, isolation,

25

30

5

10

identification, or assay of expression. In another specific embodiment, the fusion protein comprises a protease cleavage site such as a metal protease or serine cleavage site.

Construction of fusion proteins for expression in bacteria or eukaryotic systems are well known in the art and such methods are within the scope of the invention.

Any fusion protein may be readily purified by utilizing an antibody specific for the fusion protein being expressed. For example, a system described by Janknecht *et al.* (1991, *Proc. Natl. Acad. Sci. USA* 88:8972-8976) allows for the ready purification of non-denatured fusion proteins expressed in human cell lines. In this system, the nucleic acid of interest is subcloned into a vaccinia recombination plasmid such that the open reading frame is translationally fused to an amino-terminal tag consisting of six histidine residues. Extracts from cells infected with recombinant vaccinia virus are loaded onto Ni²⁺·nitriloacetic acid-agarose columns and histidine-tagged proteins are selectively eluted with imidazole-containing buffers.

5.7 ANTIBODIES GENERATED BY THE VACCINES OF THE INVENTION

Antibodies generated against mutant proteins of the invention by immunization with the vaccines formulations of the present invention also have potential uses in diagnostic assays, passive immunotherapy, and generation of antiidiotypic antibodies.

20

5

10

15

Techniques described for the production of single chain antibodies (U.S. Patent 4,946,778) can be adapted to produce single chain antibodies to immunogenic mutant polypeptide products of this invention. Also, transgenic mice may be used to express humanized antibodies to immunogenic mutant polypeptide products of this invention.

25

The vaccine formulations of the present invention can also be used to produce antibodies for use in passive immunotherapy, in which short-term protection of a host is achieved by the administration of pre-formed antibody directed against a heterologous organism.

30 fi

35

More particularly, an isolated mutant polypeptide of the invention, or a fragment thereof, can be used as an immunogen to generate antibodies using standard techniques for polyclonal and monoclonal antibody preparation. The full-length mutant polypeptide or protein can be used or, alternatively, the invention provides antigenic peptide fragments for use as immunogens. The antigenic peptide of a mutant protein of the invention comprises at least 8 (preferably 10, 15, 20, or 30) amino acid residues, and encompasses an epitope of the mutant protein such that an antibody raised against the peptide forms a specific immune complex with the protein.

Preferred epitopes encompassed by an antigenic mutant protein are regions that are located on the surface of the protein, e.g., hydrophilic regions. In certain embodiments, the nucleic acid molecules of the invention are present as part of nucleic acid molecules comprising nucleotide sequences that contain or encode heterologous (e.g., vector, expression vector, or fusion protein) sequences. These nucleotides can then be used to express proteins which can be used as immunogens to generate an immune response, or more particularly, to generate polyclonal or monoclonal antibodies specific to the expressed protein.

5

10

15

20

25

30

35

An immunogen typically is used to prepare antibodies by immunizing a suitable subject, (e.g., rabbit, goat, mouse or other mammal). An appropriate immunogenic preparation can contain, for example, recombinantly expressed or chemically synthesized mutant polypeptide. The preparation can further include an adjuvant, such as Freund's complete or incomplete adjuvant, or similar immunostimulatory agent.

Accordingly, another aspect of the invention pertains to antibodies directed against a polypeptide of the invention. The term "antibody" as used herein refers to immunoglobulin molecules and immunologically active portions of immunoglobulin molecules, *i.e.*, molecules that contain an antigen binding site which specifically binds an antigen, such as a polypeptide of the invention, *e.g.*, an epitope of a polypeptide of the invention. A molecule which specifically binds to a given polypeptide of the invention is a molecule which binds the polypeptide, but does not substantially bind other molecules in a sample, *e.g.*, a biological sample, which naturally contains the polypeptide. Examples of immunologically active portions of immunoglobulin molecules include F(ab) and F(ab')₂ fragments which can be generated by treating the antibody with an enzyme such as pepsin. The invention provides polyclonal and monoclonal antibodies. The term "monoclonal antibody" or "monoclonal antibody composition", as used herein, refers to a population of antibody molecules that contain only one species of an antigen binding site capable of immunoreacting with a particular epitope.

Polyclonal antibodies can be prepared by immunizing a suitable subject with a mutant polypeptide of the invention as an immunogen. Preferred polyclonal antibody compositions are ones that have been selected for antibodies directed against a polypeptide or polypeptides of the invention. Particularly preferred polyclonal antibody preparations are ones that contain only antibodies directed against a polypeptide or polypeptides of the invention. Particularly preferred immunogen compositions are those that contain no other human proteins such as, for example, immunogen compositions made using a non-human host cell for recombinant expression of a polypeptide of the invention. In such a manner, the

only human epitope or epitopes recognized by the resulting antibody compositions raised against this immunogen will be present as part of a polypeptide or polypeptides of the invention.

The antibody titer in the immunized subject can be monitored over time by standard techniques, such as with an enzyme linked immunosorbent assay (ELISA) using immobilized polypeptide. If desired, the antibody molecules can be isolated from the mammal (e.g., from the blood) and further purified by well-known techniques, such as protein A chromatography to obtain the IgG fraction. Alternatively, antibodies specific for a protein or polypeptide of the invention can be selected for (e.g., partially purified) or purified by, e.g., affinity chromatography. For example, a recombinantly expressed and purified (or partially purified) protein of the invention is produced as described herein, and covalently or non-covalently coupled to a solid support such as, for example, a chromatography column. The column can then be used to affinity purify antibodies specific for the proteins of the invention from a sample containing antibodies directed against a large number of different epitopes, thereby generating a substantially purified antibody composition, i.e., one that is substantially free of contaminating antibodies. By a substantially purified antibody composition is meant, in this context, that the antibody sample contains at most only 30% (by dry weight) of contaminating antibodies directed against epitopes other than those on the desired protein or polypeptide of the invention, and preferably at most 20%, yet more preferably at most 10%, and most preferably at most 5% (by dry weight) of the sample is contaminating antibodies. A purified antibody composition means that at least 99% of the antibodies in the composition are directed against the desired protein or polypeptide of the invention.

At an appropriate time after immunization, e.g., when the specific antibody titers are highest, antibody-producing cells can be obtained from the subject and used to prepare monoclonal antibodies by standard techniques, such as the hybridoma technique (originally described by Kohler and Milstein, 1975, Nature 256:495-497), the human B cell hybridoma technique (Kozbor et al., 1983, Immunol. Today 4:72), the EBV-hybridoma technique (Cole et al., 1985, Monoclonal Antibodies and Cancer Therapy, Alan R. Liss, Inc., pp. 77-96) or trioma techniques. The technology for producing hybridomas is well known (see generally Current Protocols in Immunology (1994) Coligan et al. (eds.) John Wiley & Sons, Inc., New York, NY). Hybridoma cells producing a monoclonal antibody of the invention are detected by screening the hybridoma culture supernatants for antibodies that bind the polypeptide of interest, e.g., using a standard ELISA assay.

35

30

5

10

15

20

Alternative to preparing monoclonal antibody-secreting hybridomas, a monoclonal antibody directed against a polypeptide of the invention can be identified and isolated by screening a recombinant combinatorial immunoglobulin library (e.g., an antibody phage display library) with the polypeptide of interest. Kits for generating and screening phage display libraries are commercially available (e.g., the Pharmacia Recombinant Phage Antibody System, Catalog No. 27-9400-01; and the Stratagene SurfZAP Phage Display Kit, Catalog No. 240612). Additionally, examples of methods and reagents particularly amenable for use in generating and screening antibody display library can be found in, for example, U.S. Patent No. 5,223,409; PCT Publication No. WO 92/18619; PCT Publication No. WO 91/17271; PCT Publication No. WO 92/20791; PCT Publication No. WO 92/15679; PCT Publication No. WO 93/01288; PCT Publication No. WO 92/01047; PCT Publication No. WO 92/09690; PCT Publication No. WO 90/02809; Fuchs et al., 1991, BioTechnology 9:1370-1372; Hay et al., 1992, Hum. Antibod. Hybridomas 3:81-85; Huse et al., 1989, Science 246:1275-1281; Griffiths et al., 1993, EMBO J. 12:725-734.

Additionally, recombinant antibodies, such as chimeric and humanized monoclonal antibodies, comprising both human and non-human portions, which can be made using standard recombinant DNA techniques, are within the scope of the invention. A chimeric antibody is a molecule in which different portions are derived from different animal species, such as those having a variable region derived from a murine MAB and a

5

- human immunoglobulin constant region. (See, e.g., Cabilly et al., U.S. Patent No. 4,816,567; and Boss et al., U.S. Patent No. 4,816,397, which are incorporated herein by reference in their entirety.) Humanized antibodies are antibody molecules from non-human species having one or more complementarily determining regions (CDRs) from the non-human species and a framework region from a human immunoglobulin molecule. (See, e.g., Queen, U.S. Patent No. 5,585,089, which is incorporated herein by reference in its entirety.)
- Queen, U.S. Patent No. 5,585,089, which is incorporated herein by reference in its entirety.) Such chimeric and humanized monoclonal antibodies can be produced by recombinant DNA techniques known in the art, for example using methods described in PCT Publication No. WO 87/02671; European Patent Application 184,187; European Patent Application 171,496; European Patent Application 173,494; PCT Publication No. WO 86/01533; U.S. Patent No.
- 4,816,567; European Patent Application 125,023; Better et al., 1988, Science
 240:1041-1043; Liu et al., 1987, Proc. Natl. Acad. Sci. USA 84:3439-3443; Liu et al., 1987,
 J. Immunol. 139:3521-3526; Sun et al., 1987, Proc. Natl. Acad. Sci. USA 84:214-218;
 Nishimura et al., 1987, Canc. Res. 47:999-1005; Wood et al., 1985, Nature 314:446-449;
 and Shaw et al., 1988, J. Natl. Cancer Inst. 80:1553-1559; Morrison, 1985, Science
- 35 229:1202-1207; Oi et al., 1986, BioTechniques 4:214; U.S. Patent 5,225,539; Jones et al.,

1986, Nature 321:552-525; Verhoeyan et al., 1988, Science 239:1534; and Beidler et al., 1988, J. Immunol. 141:4053-4060.

5

10

20

25

30

Completely human antibodies are particularly desirable for therapeutic treatment of human patients. Such antibodies can be produced, for example, using transgenic mice which are incapable of expressing endogenous immunoglobulin heavy and light chains genes, but which can express human heavy and light chain genes. The transgenic mice are immunized in the normal fashion with a selected antigen, e.g., all or a portion of a polypeptide of the invention. Monoclonal antibodies directed against the antigen can be obtained using conventional hybridoma technology. The human immunoglobulin transgenes harbored by the transgenic mice rearrange during B cell differentiation, and subsequently undergo class switching and somatic mutation. Thus, using such a technique, it is possible to produce therapeutically useful IgG, IgA and IgE antibodies. For an overview of this technology for producing human antibodies, see Lonberg and Huszar (1995, Int. Rev. Immunol. 13:65-93). For a detailed discussion of this technology for producing human antibodies and human monoclonal antibodies and protocols for producing such antibodies, see, e.g., U.S. Patent 5,625,126; U.S. Patent 5,633,425; U.S. Patent 5,569,825; U.S. Patent 5,661,016; and U.S. Patent 5,545,806. In addition, companies such as Abgenix, Inc. (Freemont, CA), can be engaged to provide human antibodies directed against a selected antigen using technology similar to that described above.

Completely human antibodies which recognize a selected epitope can be generated using a technique referred to as "guided selection." In this approach a selected non-human monoclonal antibody, e.g., a mouse antibody, is used to guide the selection of a completely human antibody recognizing the same epitope. (Jespers et al., 1994, BioTechnology 12:899-903).

An antibody directed against a polypeptide of the invention can be used to detect the protein (e.g., in a cellular lysate or cell supernatant) in order to evaluate the abundance and pattern of expression of the polypeptide. The antibodies can also be used diagnostically to monitor protein levels in tissue as part of a clinical testing procedure, e.g., to, for example, determine the efficacy of a given treatment regimen. Detection can be facilitated by coupling the antibody to a detectable substance. Examples of detectable substances include various enzymes, prosthetic groups, fluorescent materials, luminescent materials, bioluminescent materials, and radioactive materials. Examples of suitable enzymes include horseradish peroxidase, alkaline phosphatase, beta-galactosidase, or acetylcholinesterase; examples of suitable prosthetic group complexes include streptavidin/biotin and avidin/biotin; examples of suitable fluorescent materials include

umbelliferone, fluorescein, fluorescein isothiocyanate, rhodamine, dichlorotriazinylamine fluorescein, dansyl chloride or phycoerythrin; an example of a luminescent material includes luminol; examples of bioluminescent materials include luciferase, luciferin, and aequorin, and examples of suitable radioactive material include ¹²⁵I, ¹³¹I, ³⁵S or ³H.

5

10

In addition, gene sequences and gene products of the invention, including peptide fragments, as well as specific antibodies thereto, can be used for construction of fusion proteins to facilitate recovery, detection, or localization of another protein of interest.

Further, an antibody (or fragment thereof) may be conjugated to a therapeutic moiety such as a cytotoxin, a therapeutic agent or a radioactive metal ion. A cytotoxin or cytotoxic agent includes any agent that is detrimental to cells, and in particular, prokaryotic cells.

The conjugates of the invention can be used for modifying a given biological response, the drug moiety is not to be construed as limited to classical chemical therapeutic agents. For example, the drug moiety may be a protein or polypeptide possessing a desired biological activity. Such proteins may include, for example, a toxin such as abrin, ricin A, pseudomonas exotoxin, or diphtheria toxin; a protein such as tumor necrosis factor, α-interferon, β-interferon, nerve growth factor, platelet derived growth factor, tissue plasminogen activator, a thrombotic agent or an anti-angiogenic agent, e.g., angiostatin or endostatin; or, biological response modifiers such as, for example, lymphokines, interleukin-1 ("IL-1"), interleukin-2 ("IL-2"), interleukin-6 ("IL-6"), granulocyte macrophage colony stimulating factor ("GM-CSF"), granulocyte colony stimulating factor ("G-CSF"), interleukin-10 ("IL-10"), interleukin-12 ("IL-12"), interferon-γ ("IFN-γ"), interferon-α ("IFN-γ"), or other immune factors or growth factors.

known, see, e.g., Arnon et al., "Monoclonal Antibodies For Immunotargeting Of Drugs In Cancer Therapy", in Monoclonal Antibodies And Cancer Therapy, Reisfeld et al. (eds.), pp. 243-56 (Alan R. Liss, Inc. 1985); Hellstrom et al., "Antibodies For Drug Delivery", in Controlled Drug Delivery (2nd Ed.), Robinson et al. (eds.), pp. 623-53 (Marcel Dekker, Inc. 1987); Thorpe, "Antibody Carriers Of Cytotoxic Agents In Cancer Therapy: A Review", in Monoclonal Antibodies '84: Biological And Clinical Applications, Pinchera et al. (eds.), pp. 475-506 (1985); "Analysis, Results, And Future Prospective Of The Therapeutic Use Of Radiolabeled Antibody In Cancer Therapy", in Monoclonal Antibodies For Cancer Detection And Therapy, Baldwin et al. (eds.), pp. 303-16 (Academic Press 1985), and Thorpe et al., 1982, Immunol. Rev., 62:119-58.

An antibody with or without a therapeutic moiety conjugated to it can be used as a therapeutic that is passively administered alone or in combination with chemotherapeutic agents.

Alternatively, an antibody of the invention can be conjugated to a second antibody to form an "antibody heteroconjugate" as described by Segal in U.S. Patent No. 4,676,980 or alternatively, the antibodies can be conjugated to form an "antibody heteropolymer" as described in Taylor *et al.*, in U.S. Patent Nos. 5,470,570 and 5,487,890.

An antibody with or without a therapeutic moiety conjugated to it can be used as a therapeutic that is administered alone or in combination with cytotoxic factor(s) and/or cytokine(s).

In yet a further aspect, the invention provides substantially purified antibodies or fragments thereof, including human or non-human antibodies or fragments thereof, which antibodies or fragments specifically bind to a polypeptide of the invention. In various embodiments, the substantially purified antibodies of the invention, or fragments thereof, can be human, non-human, chimeric and/or humanized antibodies.

In another aspect, the invention provides non-human antibodies or fragments thereof. Such non-human antibodies can be goat, mouse, sheep, horse, chicken, rabbit, or rat antibodies. Alternatively, the non-human antibodies of the invention can be chimeric and/or humanized antibodies. In addition, the non-human antibodies of the invention can be polyclonal antibodies or monoclonal antibodies.

In still a further aspect, the invention provides monoclonal antibodies or fragments thereof. The monoclonal antibodies can be human, humanized, chimeric and/or non-human antibodies.

Any of the antibodies of the invention can be conjugated to a therapeutic moiety or to a detectable substance. Non-limiting examples of detectable substances that can be conjugated to the antibodies of the invention are an enzyme, a prosthetic group, a fluorescent material, a luminescent material, a bioluminescent material, and a radioactive material.

The invention also provides a kit containing an antibody of the invention conjugated to a detectable substance, and instructions for use. Still another aspect of the invention is a pharmaceutical composition comprising an antibody of the invention and a pharmaceutically acceptable carrier. In preferred embodiments, the pharmaceutical composition contains an antibody of the invention, a therapeutic moiety, and a pharmaceutically acceptable carrier.

5

10

15

20

After immunization, a sample is collected from the mammal that contains an antibody that specifically recognizes the immunogen. Preferably, the polypeptide is recombinantly produced using a non-human host cell. Optionally, the antibodies can be further purified from the sample using techniques well known to those of skill in the art. The method can further comprise producing a monoclonal antibody-producing cell from the cells of the mammal. Optionally, antibodies are collected from the antibody-producing cell.

5

10

15

20

25

30

35

5.8 RECOMBINANT METHODS OF PRODUCING ANTIBODIES

The antibodies of the invention or fragments thereof can be produced by any method known in the art for the synthesis of antibodies, in particular, by chemical synthesis or preferably, by recombinant expression techniques.

The nucleotide sequence encoding an antibody of the invention can be obtained from sequencing hybridoma clone DNA. If a clone containing a nucleic acid encoding a particular antibody or an epitope-binding fragment thereof is not available, but the sequence of the antibody molecule or epitope-binding fragment thereof is known, a nucleic acid encoding the immunoglobulin may be chemically synthesized or obtained from a suitable source (e.g., an antibody cDNA library, or a cDNA library generated from, or nucleic acid, preferably poly A+RNA, isolated from any tissue or cells expressing the antibody, such as hybridoma cells selected to express an antibody) by PCR amplification using synthetic primers hybridizable to the 3' and 5' ends of the sequence or by cloning using an oligonucleotide probe specific for the particular gene sequence to identify, e.g., a cDNA clone from a cDNA library that encodes the antibody. Amplified nucleic acids generated by PCR may then be cloned into replicable cloning vectors using any method well known in the art.

Once the nucleotide sequence of the antibody is determined, the nucleotide sequence of the antibody may be manipulated using methods well known in the art for the manipulation of nucleotide sequences, e.g., recombinant DNA techniques, site directed mutagenesis, PCR, etc. (see, for example, the techniques described in Sambrook et al., 1990, Molecular Cloning, A Laboratory Manual, 2d Ed., Cold Spring Harbor Laboratory, Cold Spring Harbor, NY; and Ausubel et al., eds., 1998, Current Protocols in Molecular Biology, John Wiley & Sons, NY, which are both incorporated by reference herein in their entireties), to generate antibodies having a different amino acid sequence by, for example, introducing amino acid substitutions, deletions, and/or insertions into the epitope-binding domain regions of the antibodies and preferably, into the hinge-Fc regions of the antibodies which are involved in the interaction with the FcRn. In a preferred embodiment, antibodies having

one or more modifications in amino acid residues 251-256, amino acid residues 285-290, amino acid residues 308-314, amino acid residues 382-386, and/or amino acid residues 428-436 are generated.

5

10

15

20

25

30

35

Recombinant expression of an antibody requires construction of an expression vector containing a nucleotide sequence that encodes the antibody. Once a nucleotide sequence encoding an antibody molecule or a heavy or light chain of an antibody, or portion thereof (preferably, but not necessarily, containing the heavy or light chain variable region) has been obtained, the vector for the production of the antibody molecule may be produced by recombinant DNA technology using techniques well known in the art. Thus, methods for preparing a protein by expressing a polynucleotide containing an antibody encoding nucleotide sequence are described herein. Methods which are well known to those skilled in the art can be used to construct expression vectors containing antibody coding sequences and appropriate transcriptional and translational control signals. These methods include, for example, in vitro recombinant DNA techniques, synthetic techniques, and in vivo genetic recombination. The invention, thus, provides replicable vectors comprising a nucleotide sequence encoding the constant region of the antibody molecule with one or more modifications in the amino acid residues involved in the interaction with the FcRn (see, e.g., PCT Publication WO 86/05807; PCT Publication WO 89/01036; U.S. Patent No. 5,122,464; Provisional Patent Application 60/254,880, filed December 12, 2000 by Johnson et al.; and Provisional Patent Application 60/289,760, filed May 9, 2001 by Johnson et al.). The nucleotide sequence encoding the heavy-chain variable region, light-chain variable region, both the heavy-chain and light-chain variable regions, an epitope-binding fragment of the heavy- and/or light-chain variable region, or one or more complementarity determining regions (CDRs) of an antibody may be cloned into such a vector for expression.

The expression vector is transferred to a host cell by conventional techniques and the transfected cells are then cultured by conventional techniques to produce an antibody having an increased affinity for the FcRn and an increased *in vivo* half-life. Thus, the invention includes host cells containing a polynucleotide encoding an antibody, an hinge-Fc region or fragments thereof (*i.e.*, constant regions) having one or more modifications in amino acid residues 251-256, amino acid residues 285-290, amino acid residues 308-314, amino acid residues 382-386, and/or amino acid residues 428-436, operably linked to a heterologous promoter.

A variety of host-expression vector systems may be utilized to express the antibody molecules of the invention. Such host-expression systems represent vehicles by which the coding sequences of interest may be produced and subsequently purified, but also

5

10

15

20

25

30

35

represent cells which may, when transformed or transfected with the appropriate nucleotide coding sequences, express an antibody molecule of the invention in situ. These include but are not limited to microorganisms such as bacteria (e.g., E. coli and B. subtilis) transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing antibody coding sequences; yeast (e.g., Saccharomyces and Pichia) transformed with recombinant yeast expression vectors containing antibody coding sequences; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing antibody coding sequences; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; and tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing antibody coding sequences; and mammalian cell systems (e.g., COS, CHO, BHK, 293, 3T3, and NS0 cells) harboring recombinant expression constructs containing promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter). Preferably, bacterial cells such as Escherichia coli, and more preferably, eukaryotic cells, especially for the expression of whole recombinant antibody molecule, are used for the expression of a recombinant antibody molecule. For example, mammalian cells such as Chinese hamster ovary cells (CHO), in conjunction with a vector such as the major intermediate early gene promoter element from human cytomegalovirus is an effective expression system for antibodies (Foecking et al., Gene, 45:101, 1986, and Cockett et al., BioTechnology, 8:2, 1990).

In bacterial systems, a number of expression vectors may be advantageously selected depending upon the use intended for the antibody molecule being expressed. For example, when a large quantity of such a protein is to be produced, for the generation of pharmaceutical compositions of an antibody molecule, vectors which direct the expression of high levels of fusion protein products that are readily purified may be desirable. Such vectors include, but are not limited to, the *E. coli* expression vector pUR278 (Ruther *et al.*, 1983, *EMBO* 12:1791), in which the antibody coding sequence may be ligated individually into the vector in frame with the lacZ coding region so that a fusion protein is produced; and pIN vectors (Inouye & Inouye, 1985, *Nucleic Acids Res.*, 13:3101-3109; Van Heeke & Schuster, 1989, *J. Biol. Chem.* 24:5503-5509).

In an insect system, Autographa californica nuclear polyhedrosis virus (AcNPV) is used as a vector to express foreign genes. The virus grows in *Spodoptera* frugiperda cells. The antibody coding sequence may be cloned individually into non-essential regions (for example the polyhedrin gene) of the virus and placed under control of

an AcNPV promoter (for example the polyhedrin promoter).

5

10

15

20

`25

30

35

In mammalian host cells, a number of viral-based expression systems may be utilized to express an antibody molecule of the invention. In cases where an adenovirus is used as an expression vector, the antibody coding sequence of interest may be ligated to an adenovirus transcription/translation control complex, e.g., the late promoter and tripartite leader sequence. This chimeric gene may then be inserted in the adenovirus genome by in vitro or in vivo recombination. Insertion in a non-essential region of the viral genome (e.g., region El or E3) will result in a recombinant virus that is viable and capable of expressing the antibody molecule in infected hosts (e.g., see Logan & Shenk, Proc. Natl. Acad. Sci. USA, 8 1:355-359, 1984). Specific initiation signals may also be required for efficient translation of inserted antibody coding sequences. These signals include the ATG initiation codon and adjacent sequences. Furthermore, the initiation codon must be in phase with the reading frame of the desired coding sequence to ensure translation of the entire insert. These exogenous translational control signals and initiation codons can be of a variety of origins, both natural and synthetic. The efficiency of expression may be enhanced by the inclusion of appropriate transcription enhancer elements, transcription terminators, etc. (see, e.g., Bitter et al., Methods in Enzymol., 153:516-544, 1987).

In addition, a host cell strain may be chosen which modulates the expression of the antibody sequences, or modifies and processes the antibody in the specific fashion desired. Such modifications (e.g., glycosylation) and processing (e.g., cleavage) of protein products may be important for the function of the antibody. Different host cells have characteristic and specific mechanisms for the post-translational processing and modification of proteins and gene products. Appropriate cell lines or host systems can be chosen to ensure the correct modification and processing of the antibody expressed. To this end, eukaryotic host cells which possess the cellular machinery for proper processing of the primary transcript, glycosylation, and phosphorylation of the gene product may be used. Such mammalian host cells include but are not limited to CHO, VERY, BHK, HeLa, COS, MDCK, 293, 3T3, W138, NS0 and in particular, breast cancer cell lines such as, for example, BT483, Hs578T, HTB2, BT2O and T47D, and normal mammary gland cell line such as, for example, CRL7O3O and HsS78Bst.

For long-term, high-yield production of recombinant antibodies, stable expression is preferred. For example, cell lines which stably express the antibody molecule may be engineered. Rather than using expression vectors which contain viral origins of replication, host cells can be transformed with DNA controlled by appropriate expression control elements (*e.g.*, promoter, enhancer, sequences, transcription terminators,

polyadenylation sites, etc.), and a selectable marker. Following the introduction of the foreign DNA, engineered cells may be allowed to grow for 1-2 days in an enriched media, and then are switched to a selective media. The selectable marker in the recombinant plasmid confers resistance to the selection and allows cells to stably integrate the plasmid into their chromosomes and grow to form foci which in turn can be cloned and expanded into cell lines. This method may advantageously be used to engineer cell lines which express the antibody molecule. Such engineered cell lines may be particularly useful in screening and evaluation of compositions that interact directly or indirectly with the antibody molecule.

5

35

10 A number of selection systems may be used, including but not limited to, the herpes simplex virus thymidine kinase (Wigler et al., Cell, 11:223, 1977), hypoxanthine guanine phosphoribosyltransferase (Szybalska & Szybalski, Proc. Natl. Acad. Sci. USA. 48:202, 1992), and adenine phosphoribosyltransferase (Lowy et al., Cell, 22:8-17, 1980) genes can be employed in tk-, hgprt- or aprt- cells, respectively. Also, antimetabolite 15 resistance can be used as the basis of selection for the following genes: dhfr, which confers resistance to methotrexate (Wigler et al., Proc. Natl. Acad. Sci. USA, 77:357, 1980 and O'Hare et al., Proc. Natl. Acad. Sci. USA, 78:1527, 1981); gpt, which confers resistance to mycophenolic acid (Mulligan & Berg, Proc. Natl. Acad. Sci. USA, 78:2072, 1981); neo, which confers resistance to the aminoglycoside G-418 (Wu and Wu, Biotherapy, 3:87-95, 20 1991; Tolstoshev, Ann. Rev. Pharmacol. Toxicol., 32:573-596, 1993; Mulligan, Science, 260:926-932, 1993; and Morgan and Anderson, Ann. Rev. Biochem., 62: 191-217, 1993; and May, TIB TECH, 11(5):155-2 15, 1993); and hygro, which confers resistance to hygromycin (Santerre et al., Gene, 30:147, 1984). Methods commonly known in the art of recombinant DNA technology may be routinely applied to select the desired recombinant clone, and such 25 methods are described, for example, in Ausubel et al. (eds.), 1993, Current Protocols in Molecular Biology, John Wiley & Sons, NY; Kriegler, 1990, Gene Transfer and Expression, A Laboratory Manual, Stockton Press, NY; in Chapters 12 and 13, Dracopoli et al. (eds), 1994, Current Protocols in Human Genetics, John Wiley & Sons, NY; and Colberre-Garapin et al., J. Mol. Biol., 150:1, 1981, which are incorporated by reference herein in their 30 entireties.

The expression levels of an antibody molecule can be increased by vector amplification (for a review, see Bebbington and Hentschel, 1987, The use of vectors based on gene amplification for the expression of cloned genes in mammalian cells in DNA cloning, Vol.3. Academic Press, New York). When a marker in the vector system expressing antibody is amplifiable, increase in the level of inhibitor present in culture of host

cell will increase the number of copies of the marker gene. Since the amplified region is associated with the antibody gene, production of the antibody will also increase (Crouse et al., 1983, Mol. Cell. Biol., 3:257).

5

10

15

20

35

The host cell may be co-transfected with two expression vectors of the invention, the first vector encoding a heavy chain derived polypeptide and the second vector encoding a light chain derived polypeptide. The two vectors may contain identical selectable markers which enable equal expression of heavy and light chain polypeptides. Alternatively, a single vector may be used which encodes, and is capable of expressing, both heavy and light chain polypeptides. In such situations, the light chain should be placed before the heavy chain to avoid an excess of toxic free heavy chain (Proudfoot, *Nature*, 322:52, 1986; and Kohler, *Proc. Natl. Acad. Sci. USA*, 77:2 197, 1980). The coding sequences for the heavy and light chains may comprise cDNA or genomic DNA.

Once an antibody molecule of the invention has been produced by recombinant expression, it may be purified by any method known in the art for purification of an immunoglobulin molecule, for example, by chromatography (e.g., ion exchange, affinity, particularly by affinity for the specific antigen after Protein A purification, and sizing column chromatography), centrifugation, differential solubility, or by any other standard techniques for the purification of proteins. Further, the antibodies of the present invention or fragments thereof may be fused to heterologous polypeptide sequences described herein or otherwise known in the art to facilitate purification.

5.8.1 ANTIBODY CONJUGATES

The present invention encompasses antibodies recombinantly fused or chemically conjugated (including both covalently and non-covalently conjugations) to

25 heterologous polypeptides (*i.e.*, an unrelated polypeptide; or portion thereof, preferably at least 10, at least 20, at least 30, at least 40, at least 50, at least 60, at least 70, at least 80, at least 90 or at least 100 amino acids of the polypeptide) to generate fusion proteins. The fusion does not necessarily need to be direct, but may occur through linker sequences.

Antibodies fused or conjugated to heterologous polypeptides may also be used in *in vitro* immunoassays and purification methods using methods known in the art. See *e.g.*, PCT publication Number WO 93/2 1232; EP 439,095; Naramura *et al.*, 1994, *Immunol. Lett.*, 39:91-99; U.S. Patent 5,474,981; Gillies *et al.*, 1992, *Proc. Natl. Acad. Sci. USA*, 89:1428-1432; and Fell *et al.*, 1991, *J. Immunol.*, 146:2446-2452, which are incorporated herein by reference in their entireties.

Antibodies can be fused to marker sequences, such as a peptide to facilitate

purification. In preferred embodiments, the marker amino acid sequence is a hexa-histidine peptide, such as the tag provided in a pQE vector (QIAGEN, Inc.), among others, many of which are commercially available. As described in Gentz et al., 1989, Proc. Natl. Acad. Sci. USA 86:821-824, for instance, hexa-histidine provides for convenient purification of the fusion protein. Other peptide tags useful for purification include, but are not limited to, the hemagglutinin "HA" tag, which corresponds to an epitope derived from the influenza hemagglutinin protein (Wilson et al., 1984, Cell, 37:767) and the "flag" tag (Knappik et al., 1994, BioTechniques, 17:754-761).

5

The present invention also encompasses antibodies conjugated to a diagnostic 10 or therapeutic agent or any other molecule for which serum half-life is desired to be increased. The antibodies can be used diagnostically to, for example, monitor the development or progression of a disease, disorder or infection as part of a clinical testing procedure to, e.g., determine the efficacy of a given treatment regimen. Detection can be facilitated by coupling the antibody to a detectable substance. Examples of detectable 15 substances include various enzymes, prosthetic groups, fluorescent materials, luminescent materials, bioluminescent materials, radioactive materials, positron emitting metals, and nonradioactive paramagnetic metal ions. The detectable substance may be coupled or conjugated either directly to the antibody or indirectly, through an intermediate (such as, for example, a linker known in the art) using techniques known in the art. See, for example, 20 U.S. Patent No. 4,741,900 for metal ions which can be conjugated to antibodies for use as diagnostics according to the present invention. Examples of suitable enzymes include horseradish peroxidase, alkaline phosphatase, beta-galactosidase, or acetylcholinesterase; examples of suitable prosthetic group complexes include streptavidin/biotin and avidin/biotin; examples of suitable fluorescent materials include umbelliferone, fluorescein, 25 fluorescein isothiocyanate, rhodamine, dichlorotriazinylamine fluorescein, dansyl chloride or phycoerythrin; an example of a luminescent material includes luminol; examples of bioluminescent materials include luciferase, luciferin, and aequorin; and examples of suitable radioactive material include ¹²⁵I, ¹³¹I, ¹¹¹In or ⁹⁹Tc.

An antibody may be conjugated to a therapeutic moiety such as a cytotoxin

(e.g., a cytostatic or cytocidal agent), a therapeutic agent or a radioactive element (e.g., alpha-emitters, gamma-emitters, etc.). Cytotoxins or cytotoxic agents include any agent that is detrimental to cells. Examples include paclitaxol, cytochalasin B, gramicidin D, ethidium bromide, emetine, mitomycin, etoposide, tenoposide, vincristine, vinblastine, colchicin, doxorubicin, daunorubicin, dihydroxy anthracin dione, mitoxantrone, mithramycin,

actinomycin D, 1-dehydrotestosterone, glucocorticoids, procaine, tetracaine, lidocaine,

PCT/US01/47994 WO 02/102974

propranolol, and puromycin and analogs or homologs thereof. Therapeutic agents include, but are not limited to, antimetabolites (e.g., methotrexate, 6-mercaptopurine, 6-thioguanine, cytarabine, 5-fluorouracil decarbazine), alkylating agents (e.g., mechlorethamine, thioepa chlorambucil, melphalan, carmustine (BSNU) and lomustine (CCNU), cyclothosphamide, busulfan, dibromomannitol, streptozotocin, mitomycin C, and cisdichlorodiamine platinum (II) (DDP) cisplatin), anthracyclines (e.g., daunorubicin (formerly daunomycin) and doxorubicin), antibiotics (e.g., dactinomycin (formerly actinomycin), bleomycin, mithramycin, and anthramycin (AMC)), and anti-mitotic agents (e.g., vincristine and vinblastine).

10

15

20

5

Further, an antibody may be conjugated to a therapeutic agent or drug moiety that modifies a given biological response. Therapeutic agents or drug mojeties are not to be construed as limited to classical chemical therapeutic agents. For example, the drug moiety may be a protein or polypeptide possessing a desired biological activity. Such proteins may include, for example, a toxin such as abrin, ricin A, pseudomonas exotoxin, or diphtheria toxin; a protein such as tumor necrosis factor, α -interferon (IFN- α), β -interferon (IFN- β), nerve growth factor (NGF), platelet derived growth factor (PDGF), tissue plasminogen activator (TPA), an apoptotic agent (e.g., TNF-α, TNF-β, AIM I as disclosed in PCT Publication No. WO 97/33899), AIM II (see, PCT Publication No. WO 97/34911), Fas Ligand (Takahashi et al., 1994, J. Iminunol., 6:1567-1574), and VEGI (PCT Publication No. WO 99/23105), a thrombotic agent or an anti-angiogenic agent (e.g., angiostatin or endostatin); or a biological response modifier such as, for example, a lymphokine (e.g., interleukin-1 ("IL-1"), interleukin-2 ("IL-2"), interleukin-6 ("IL-6"), granulocyte macrophage colony stimulating factor ("GM-CSF"), and granulocyte colony stimulating factor ("G-CSF"), or a growth factor (e.g., growth hormone ("GH")).

25

30

Techniques for conjugating such therapeutic moieties to antibodies are well known; see, e.g., Arnon et al., "Monoclonal Antibodies For Immunotargeting Of Drugs In Cancer Therapy", in Monoclonal Antibodies And Cancer Therapy, Reisfeld et al. (eds.), 1985, pp. 243-56, Alan R. Liss, Inc.); Hellstrom et al., "Antibodies For Drug Delivery", in Controlled Drug Delivery (2nd Ed.), Robinson et al. (eds.), 1987, pp. 623-53, Marcel Dekker, Inc.); Thorpe, "Antibody Carriers Of Cytotoxic Agents In Cancer Therapy: A Review", in Monoclonal Antibodies '84: Biological And Clinical Applications, Pinchera et al. (eds.), 1985, pp. 475-506); "Analysis, Results, And Future Prospective Of The Therapeutic Use Of Radiolabeled Antibody In Cancer Therapy", in Monoclonal Antibodies For Cancer Detection And Therapy, Baldwin et al. (eds.), 1985, pp. 303-16, Academic

35 Press; and Thorpe et al., 1982, Immunol. Rev., 62:119-58.

An antibody or fragment thereof, with or without a therapeutic moiety conjugated to it, administered alone or in combination with cytotoxic factor(s) and/or cytokine(s) can be used as a therapeutic.

5

10

20

25

30

35

Alternatively, an antibody can be conjugated to a second antibody to form an antibody heteroconjugate as described by Segal in U.S. Patent No. 4,676,980, which is incorporated herein by reference in its entirety.

Antibodies may also be attached to solid supports, which are particularly useful for immunoassays or purification of the target antigen. Such solid supports include, but are not limited to, glass, cellulose, polyacrylamide, nylon, polystyrene, polyvinyl chloride or polypropylene.

5.9 Crystal Structure

5.9.1 Crystalline FimCH

In another aspect, the present invention provides co-crystals of FimCH complexes with a mannose sugar, the crystal structures derived therefrom and methods of their use.

In the co-crystals, the mannose sugar can be any mannose sugar including, for example, mannopentanose, methyl-alpha-D-mannopyranoside, alpha-D-mannopyranoside, mannotriose, an oligomannoside, a dimannoside, etc.

The crystals from which the atomic structure coordinates of the invention may be obtained include native crystals and heavy-atom derivative crystals. Native crystals generally comprise substantially pure polypeptides corresponding to FimCH in crystalline form.

It is to be understood that the crystalline FimCH from which the atomic structure coordinates of the invention can be obtained is not limited to wild-type FimCH. Indeed, the crystals may comprise mutants of wild-type FimCH. Mutants of wild-type FimCH are obtained by replacing at least one amino acid residue in the sequence of the wild-type FimCH with a different amino acid residue, or by adding or deleting one or more amino acid residues within the wild-type sequence and/or at the – and/or C-terminus of the wild-type FimCH.

The types of mutants contemplated by this invention include conservative mutants, non-conservative mutants, deletion mutants, truncated mutants, extended mutants, methionine mutants, selenomethionine mutants, cysteine mutants and selenocysteine mutants. A mutant may have, but need not have, FimCH activity. Methionine, selenomethione, cysteine, and selenocysteine mutants are particularly useful for producing

heavy-atom derivative crystals, as described in detail, below.

5

10

15

20

25

30

35

It will be recognized by one of skill in the art that the types of mutants contemplated herein are not mutually exclusive; that is, for example, a polypeptide having a conservative mutation in one amino acid may in addition have several Leu or Ile to Met mutations.

The amino acid residue Cys (C) is unusual in that it can form disulfide bridges with other Cys (C) residues or other sulfhydryl-containing amino acids ("cysteine-like amino acids"). The ability of Cys (C) residues and other cysteine-like amino acids to exist in a polypeptide in either the reduced free -SH or oxidized disulfide-bridged form affects whether Cys (C) residues contribute net hydrophobic or hydrophilic character to a polypeptide. While Cys (C) exhibits a hydrophobicity of 0.29 according to the consensus scale of Eisenberg *et al.* (1984, J. *Mol. Biol.* 179:125-142.), it is to be understood that for purposes of the present invention Cys (C) is categorized as a polar hydrophilic amino acid, notwithstanding the general classifications defined above. Preferably, Cys residues that are known to participate in disulfide bridges are not substituted or are conservatively substituted with other cysteine-like amino acids so that the residue can participate in a disulfide bridge. Typical cysteine-like residues include, for example, Pen, hCys, etc. Substitutions for Cys residues that interfere with crystallization are discussed *infra*.

While in most instances the amino acids of FimCH will be substituted with genetically-encoded amino acids, in certain circumstances mutants may include genetically non-encoded amino acids. For example, non-encoded derivatives of certain encoded amino acids, such as SeMet and/or SeCys, may be incorporated into the polypeptide chain using biological expression systems (such SeMet and SeCys mutants are described in more detail, *infra*).

Alternatively, in instances where the mutant will be prepared in whole or in part by chemical synthesis, virtually any non-encoded amino acids may be used, ranging from D-isomers of the genetically encoded amino acids to non-encoded naturally-occurring natural and synthetic amino acids.

Conservative amino acid substitutions for many of the commonly known non-genetically encoded amino acids are well known in the art. Conservative substitutions for other non-encoded amino acids can be determined based on their physical properties as compared to the properties of the genetically encoded amino acids.

In some instances, it may be particularly advantageous or convenient to substitute, delete from and/or add amino acid residues to FimCH in order to provide convenient cloning sites in cDNA encoding the polypeptide, to aid in purification of the

polypeptide, etc. Such substitutions, deletions and/or additions that do not substantially alter the three dimensional structure of the native FimCH will be apparent to those having skills in the art. These substitutions, deletions and/or additions include, but are not limited to, His tags, intein-containing self-cleaving tags, maltose binding protein fusions, glutathione Stransferase protein fusions, antibody fusions, green fluorescent protein fusions, signal peptide fusions, biotin accepting peptide fusions, and the like.

Mutations may also be introduced into a polypeptide sequence where there are residues, e.g., cysteine residues, that interfere with crystallization. Such cysteine residues can be substituted with an appropriate amino acid that does not readily form covalent bonds with other amino acid residues under crystallization conditions; e.g., by substituting the cysteine with Ala, Ser or Gly. Any cysteine located in a non-helical or non- β -stranded segment, based on secondary structure assignments, are good candidates for replacement.

It should be noted that the mutants contemplated herein need not exhibit FimCH activity. Indeed, amino acid substitutions, additions or deletions that interfere with the activity of FimCH are specifically contemplated by the invention. Such crystalline polypeptides, or the atomic structure coordinates obtained therefrom, can be used to provide phase information to aid the determination of the three-dimensional X-ray structures of other related or non-related crystalline polypeptides.

20

5

The heavy-atom derivative crystals from which the atomic structure coordinates of the invention are obtained generally comprise a crystalline FimCH polypeptide in association with one or more heavy metal atoms. The polypeptide may correspond to a wild-type or a mutant FimCH, which may optionally be in co-complex with one or more molecules, as previously described. There are two types of heavy-atom derivatives of polypeptides: heavy-atom derivatives resulting from exposure of the protein to a heavy metal in solution, wherein crystals are grown in medium comprising the heavy metal, or in crystalline form, wherein the heavy metal diffuses into the crystal, and heavy-atom derivatives wherein the polypeptide comprises heavy-atom containing amino acids, e.g., selenomethionine and/or selenocysteine mutants.

30

35

25

In practice, heavy-atom derivatives of the first type can be formed by soaking a native crystal in a solution comprising heavy metal atom salts, or organometallic compounds, e.g., lead chloride, gold thiomalate, ethylmercurithiosalicylic acid-sodium salt (thimerosal), uranyl acetate, platinum tetrachloride, osmium tetraoxide, zinc sulfate, and cobalt hexamine, which can diffuse through the crystal and bind to the crystalline polypeptide.

Heavy-atom derivatives of this type can also be formed by adding to a crystallization solution comprising the polypeptide to be crystallized an amount of a heavy metal atom salt, which may associate with the protein and be incorporated into the crystal. The location(s) of the bound heavy metal atom(s) can be determined by X-ray diffraction analysis of the crystal. This information, in turn, is used to generate the phase information needed to construct the three-dimensional structure of the protein.

5

10

15

20

25

30

35

Heavy-atom derivative crystals may also be prepared from polypeptides that include one or more SeMet and/or SeCys residues (SeMet and/or SeCys mutants). Such selenocysteine or selenomethionine mutants may be made from wild-type or mutant FimCH by expression of FimCH-encoding cDNAs in auxotrophic E. coli strains. Hendrickson et al., 1990, EMBO J. 9(5):1665-1672. In this method, the wild-type or mutant FimCH cDNA may be expressed in a host organism on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both). Alternatively, selenocysteine or selenomethionine mutants may be made using nonauxotrophic E. coli strains, e.g., by inhibiting methionine biosynthesis in these strains with high concentrations of Ile, Lys, Phe, Leu, Val or Thr and then providing selenomethionine in the medium (Doublié, 1997, Methods in Enzymology 276:523-530). Furthermore, selenocysteine can be selectively incorporated into polypeptides by exploiting the prokaryotic and eukaryotic mechanisms for selenocysteine incorporation into certain classes of proteins in vivo, as described in U.S. Patent No. 5,700,660 to Leonard et al. (filed June 7, 1995). One of skill in the art will recognize that selenocysteine is preferably not incorporated in place of cysteine residues that form disulfide bridges, as these may be important for maintaining the three-dimensional structure of the protein and are preferably not to be eliminated. One of skill in the art will further recognize that, in order to obtain accurate phase information, approximately one selenium atom should be incorporated for every 140 amino acid residues of the polypeptide chain. The number of selenium atoms incorporated into the polypeptide chain can be conveniently controlled by designing a Met or Cys mutant having an appropriate number of Met and/or Cys residues, as described more fully below.

In some instances, the polypeptide to be crystallized may not contain cysteine or methionine residues. Therefore, if selenomethionine and/or selenocysteine mutants are to be used to obtain heavy-atom derivative crystals, methionine and/or cysteine residues may be introduced into the polypeptide chain. Likewise, Cys residues must be introduced into the polypeptide chain if the use of a cysteine-binding heavy metal, such as mercury, is contemplated for production of a heavy-atom derivative crystal.

Such mutations are preferably introduced into the polypeptide sequence at sites that will not disturb the overall protein fold. For example, a residue that is conserved among many members of the protein family or that is thought to be involved in maintaining its activity or structural integrity, as determined by, e.g., sequence alignments, should not be mutated to a Met or Cys. In addition, conservative mutations, such as Ser to Cys, or Leu or lle to Met, are preferably introduced. One additional consideration is that, in order for a heavy-atom derivative crystal to provide phase information for structure determination, the location of the heavy atom(s) in the crystal unit cell must be determinable and provide phase information. Therefore, a mutation is preferably not introduced into a portion of the protein that is likely to be mobile, e.g., at, or within about 1-5 residues of, the — and C-termini.

5

10

15

20

25

30

35

Conversely, if there are too many methionine and/or cysteine residues in a polypeptide sequence, over-incorporation of the selenium-containing side chains can lead to the inability of the polypeptide to fold and/or crystallize, and may potentially lead to complications in solving the crystal structure. In this case, methionine and/or cysteine mutants are prepared by substituting one or more of these Met and/or Cys residues with another residue. The considerations for these substitutions are the same as those discussed above for mutations that introduce methionine and/or cysteine residues into the polypeptide. Specifically, the Met and/or Cys residues are preferably conservatively substituted with Leu/Ile and Ser, respectively.

As DNA encoding cysteine and methionine mutants can be used in the methods described above for obtaining SeCys and SeMet heavy-atom derivative crystals, the preferred Cys or Met mutant will have one Cys or Met residue for every 140 amino acids.

5.9.2 Crystallization Of Polypeptides And Characterization Of Crystals

The native, heavy-atom derivative and co-crystals from which the atomic structure coordinates of the invention are obtained can be obtained by conventional means as are well-known in the art of protein crystallography, including batch, liquid bridge, dialysis, and vapor diffusion methods (see, e.g., McPherson, 1998, 'Crystallization of Biological Macromolecules', Cold Spring Harbor Press, New York; McPherson, 1990, Eur. J. Biochem. 189:1-23.; Weber, 1991, Adv. Protein Chem. 41:1-36.).

Generally, native crystals are grown by dissolving substantially pure FimCH polypeptide complex in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Examples of precipitants include, but are not limited to, polyethylene glycol, ammonium sulfate, 2-methyl-2,4-pentanediol, sodium

citrate, sodium chloride, glycerol, isopropanol, lithium sulfate, sodium acetate, sodium formate, potassium sodium tartrate, ethanol, hexanediol, ethylene glycol, dioxane, t-butanol and combinations thereof. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

5

10

35

weeks, until crystals grow.

In a preferred embodiment, native crystals are grown by vapor diffusion in sitting drops (McPherson, 1982, "Preparation and Analysis of Protein Crystals", John Wiley, New York; McPherson, 1990, Eur. J. Biochem. 189:1-23). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 25 µl of substantially pure polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. The sealed container is allowed to stand, usually for about 2-6

In one embodiment of the invention, native co-crystals of a wild type FimCH alpha-D-mannopyranoside complex from which atomic structure coordinates of the invention are obtained, can be obtained by the hanging drop method or by the sitting drop method. About 6 ul of FimCH polypeptide (4.7 mg/ml in 100 mMTris-HCl, pH 8.2, and 7 mM alpha-D-mannopyranoside) and 6 ul reservoir solution (0.7 M ammonium sulfate and 100 mM Tris-HCl, pH 8.2) suspended over 0.5 ml reservoir solution for about 3 to 4 weeks at 20°C provide diffraction quality crystals. The buffer solution optionally can be raised to 0.9 to 1.2 M ammonium sulfate after about two days, and the crystallization solution can be optionally microseeded with, for example, a cat whisker after one week to improve crystallization.

25 Q133N methyl-alpha-D-mannopyranoside complex from which atomic structure coordinates of the invention are obtained, can be obtained by the hanging drop method or by the sitting drop method. About 6 ul of FimCH Q133N complex (4.7 mg/ml in 100 mM Tris-HCl, pH 8.2, and 10 mM methyl-alpha-D-mannopyranoside) and 6 ul reservoir solution (0.7 M ammonium sulfate and 100 mM Tris-HCl, pH 8.2) suspended over 0.5 ml reservoir solution for about 3 to 4 weeks at 20°C provide diffraction quality crystals. The buffer solution optionally can be raised to 0.9 to 1.2 M ammonium sulfate after about two days, and the crystallization solution can be optionally microseeded with, for example, a cat whisker after one week to improve crystallization.

Of course, those having skill in the art will recognize that the abovedescribed crystallization conditions can be varied. Such variations may be used alone or in

combination, and include polypeptide solutions containing polypeptide concentrations between 0.06 to 0.12 mM, alpha-D-mannopyranoside or methyl-alpha-D-mannopyranoside concentrations between 0.5 and 30 mM, Tris-HCl concentrations between 50 mM and 100 mM, pH ranges between 7.8 and 8.6; and reservoir solutions containing ammonium sulfate concentrations between 0.6 M and 1.2 M, Tris-HCl concentrations between 50 mM and 100 mM, pH ranges between 7.8 and 8.6 and temperature ranges between 18 °C and 24 °C. Other buffer solutions may be used such as Hepes buffer, so long as the desired pH range is maintained.

10

5

15

20

25

Heavy-atom derivative crystals can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. Heavy-atom derivative crystals can also be obtained from SeMet and/or SeCys mutants, as described above for native crystals.

Mutant complexes other than those discussed above may crystallize under slightly different crystallization conditions than wild-type protein, or under very different crystallization conditions, depending on the nature of the mutation, and its location in the protein. For example, a non-conservative mutation may result in alteration of the hydrophilicity of the mutant, which may in turn make the mutant protein either more soluble or less soluble than the wild-type protein. Typically, if a protein becomes more hydrophilic as a result of a mutation, it will be more soluble than the wild-type protein in an aqueous solution and a higher precipitant concentration will be needed to cause it to crystallize. Conversely, if a protein becomes less hydrophilic as a result of a mutation, it will be less soluble in an aqueous solution and a lower precipitant concentration will be needed to cause it to crystallize. If the mutation happens to be in a region of the protein involved in crystal lattice contacts, crystallization conditions may be affected in more unpredictable ways.

35

Co-crystals can also be obtained by soaking a native crystal in mother liquor containing compound that binds FimCH, or by co-crystallizing FimCH in the presence of one or more binding compounds, as discussed above.

5

5.9.3 Characterization of Crystals

The dimensions of a unit cell of a crystal are defined by six numbers, the lengths of three unique edges, a, b, and c, and three unique angles, α , β , and γ . The type of unit cell that comprises a crystal is dependent on the values of these variables, as discussed above in Section 3.2.

10

15

20

When a crystal is placed in an X-ray beam, the incident X-rays interact with the electron cloud of the molecules that make up the crystal, resulting in X-ray scatter. The combination of X-ray scatter with the lattice of the crystal gives rise to nonuniformity of the scatter; areas of high intensity are called diffracted X-rays. The angle at which diffracted beams emerge from the crystal can be computed by treating diffraction as if it were reflection from sets of equivalent, parallel planes of atoms in a crystal (Bragg's Law). The most obvious sets of planes in a crystal lattice are those that are parallel to the faces of the unit cell. These and other sets of planes can be drawn through the lattice points. Each set of planes is identified by three indices, hkl. The h index gives the number of parts into which the a edge of the unit cell is cut, the k index gives the number of parts into which the b edge of the unit cell is cut, and the l index gives the number of parts into which the c edge of the unit cell is cut by the set of hkl planes. Thus, for example, the 235 planes cut the a edge of each unit cell into halves, the b edge of each unit cell into thirds, and the c edge of each unit cell into fifths. Planes that are parallel to the bc face of the unit cell are the 100 planes; planes that are parallel to the ac face of the unit cell are the 010 planes; and planes that are parallel to the ab face of the unit cell are the 001 planes.

25

When a detector is placed in the path of the diffracted X-rays, in effect cutting into the sphere of diffraction, a series of spots, or reflections, are recorded to produce a "still" diffraction pattern. Each reflection is the result of X-rays reflecting off one set of parallel planes, and is characterized by an intensity, which is related to the distribution of molecules in the unit cell, and hkl indices, which correspond to the parallel planes from which the beam producing that spot was reflected. If the crystal is rotated about an axis perpendicular to the X-ray beam, a large number of reflections is recorded on the detector, resulting in a diffraction pattern.

35

30

The unit cell dimensions and space group of a crystal can be determined from its diffraction pattern. First, the spacing of reflections is inversely proportional to the

lengths of the edges of the unit cell. Therefore, if a diffraction pattern is recorded when the X-ray beam is perpendicular to a face of the unit cell, two of the unit cell dimensions may be deduced from the spacing of the reflections in the x and y directions of the detector, the crystal-to-detector distance, and the wavelength of the X-rays. Those of skill in the art will appreciate that, in order to obtain all three unit cell dimensions, the crystal must be rotated such that the X-ray beam is perpendicular to another face of the unit cell. Second, the angles of a unit cell can be determined by the angles between lines of spots on the diffraction pattern. Third, the absence of certain reflections and the repetitive nature of the diffraction pattern, which may be evident by visual inspection, indicate the internal symmetry, or space group, of the crystal. Therefore, a crystal may be characterized by its unit cell and space group, as well as by its diffraction pattern.

Once the dimensions of the unit cell are determined, the likely number of polypeptides in the asymmetric unit can be deduced from the size of the polypeptide, the density of the average protein, and the typical solvent content of a protein crystal, which is usually in the range of 30-70% of the unit cell volume (Matthews, 1968, J. *Mol. Biol.* 33:491-497).

The FimCH crystals of the present invention are generally characterized by a diffraction pattern. The crystals are further characterized by unit cell dimensions and space group symmetry information obtained from the diffraction patterns, as described above. The wild type FimCH alpha-D-mannopyranoside co-crystals and the FimCH Q133N methylalpha-D-mannopyranoside co-crystals, have a c-centered monoclinic unit cell and space group symmetry C2.

Several forms of crystalline FimCH were obtained. In the wild type FimCH alpha-D-mannopyranoside co-crystals, the unit cell has dimensions of a=138.077+/-0.2 Å, b=138.130+/-0.2 Å, c=215.352+/-0.2 Å, α =90, β =90.005, γ =90. In the FimCH Q133N methyl-alpha-D-mannopyranoside co-crystals, the unit cell has dimensions of a=138.35+/-0.2 Å, b=138.334+/- 0.2 Å, c=213.212+/- 0.2 Å and β =89.983°+/- 0.2°. There are likely to be 8FimCH molecules in the asymmetric unit in both crystalline forms, related by an approximate four-fold axis.

5.9.4 Collection of Data and Determination of Structure Solutions

The diffraction pattern is related to the three-dimensional shape of the molecule by a Fourier transform. The process of determining the solution is in essence a refocusing of the diffracted X-rays to produce a three-dimensional image of the molecule in

35

5

10

15

20

25

the crystal. Since re-focusing of X-rays cannot be done with a lens at this time, it is done via mathematical operations.

The sphere of diffraction has symmetry that depends on the internal symmetry of the crystal, which means that certain orientations of the crystal will produce the same set of reflections. Thus, a crystal with high symmetry has a more repetitive diffraction pattern, and there are fewer unique reflections that need to be recorded in order to have a complete representation of the diffraction. The goal of data collection, a data set, is a set of consistently measured, indexed intensities for as many reflections as possible. A complete data set is collected if at least 80%, preferably at least 90%, most preferably at least 95% of unique reflections are recorded. In one embodiment, a complete data set is collected using one crystal. In another embodiment, a complete data set is collected using more than one crystal of the same type.

5

10

15

20

25

30

35

Sources of X-rays include, but are not limited to, a rotating anode X-ray generator such as a Rigaku RU-200 or a beamline at a synchrotron light source, such as the Advanced Photon Source at Argonne National Laboratory. Suitable detectors for recording diffraction patterns include, but are not limited to, X-ray sensitive film, multiwire area detectors, image plates coated with phosphorus, and CCD cameras. Typically, the detector and the X-ray beam remain stationary, so that, in order to record diffraction from different parts of the crystal's sphere of diffraction, the crystal itself is moved via an automated system of moveable circles called a goniostat.

One of the biggest problems in data collection, particularly from macromolecular crystals having a high solvent content, is the rapid degradation of the crystal in the X-ray beam. In order to slow the degradation, data is often collected from a crystal at liquid nitrogen temperatures. In order for a crystal to survive the initial exposure to liquid nitrogen, the formation of ice within the crystal must be prevented by the use of a cryoprotectant. Suitable cryoprotectants include, but are not limited to, low molecular weight polyethylene glycols, ethylene glycol, sucrose, glycerol, xylitol, and combinations thereof. Crystals may be soaked in a solution comprising the one or more cryoprotectants prior to exposure to liquid nitrogen, or the one or more cryoprotectants may be added to the crystallization solution. Data collection at liquid nitrogen temperatures may allow the collection of an entire data set from one crystal.

Once a data set is collected, the information is used to determine the threedimensional structure of the molecule in the crystal. However, this cannot be done from a single measurement of reflection intensities because certain information, known as phase information, is lost between the three-dimensional shape of the molecule and its Fourier

transform, the diffraction pattern. This phase information must be acquired by methods described below in order to perform a Fourier transform on the diffraction pattern to obtain the three-dimensional structure of the molecule in the crystal. It is the determination of phase information that in effect refocuses X-rays to produce the image of the molecule.

5

One method of obtaining phase information is by isomorphous replacement, in which heavy-atom derivative crystals are used. In this method, the positions of heavy atoms bound to the molecules in the heavy-atom derivative crystal are determined, and this information is then used to obtain the phase information necessary to elucidate the three-dimensional structure of a native crystal. (Blundel *et al.*, 1976, Protein Crystallography, Academic Press).

10

15

Another method of obtaining phase information is by molecular replacement, which is a method of calculating initial phases for a new crystal of a polypeptide whose structure coordinates are unknown by orienting and positioning a polypeptide whose structure coordinates are known within the unit cell of the new crystal so as to best account for the observed diffraction pattern of the new crystal. Phases are then calculated from the oriented and positioned polypeptide and combined with observed amplitudes to provide an approximate Fourier synthesis of the structure of the molecules comprising the new crystal. (Lattman, 1985, *Methods in Enzymology* 115:55-77; Rossmann, 1972, "The Molecular Replacement Method," Int. Sci. Rev. Ser. No. 13, Gordon & Breach, New York).

20

25

A third method of phase determination is multi-wavelength anomalous diffraction or MAD. In this method, X-ray diffraction data are collected at several different wavelengths from a single crystal containing at least one heavy atom with absorption edges near the energy of incoming X-ray radiation. The resonance between X-rays and electron orbitals leads to differences in X-ray scattering that permits the locations of the heavy atoms to be identified, which in turn provides phase information for a crystal of a polypeptide. A detailed discussion of MAD analysis can be found in Hendrickson, 1985, *Trans. Am. Crystallogr. Assoc.*, 21:11; Hendrickson *et al.*, 1990, *EMBO J. 9*:1665; and Hendrickson, 1991, *Science* 4:91.

30

A fourth method of determining phase information is single wavelength anomalous dispersion or SAD. In this technique, X-ray diffraction data are collected at a single wavelength from a single native or heavy-atom derivative crystal, and phase information is extracted using anomalous scattering information from atoms such as sulfur or chlorine in the native crystal or from the heavy atoms in the heavy-atom derivative crystal. The wavelength of X-rays used to collect data for this phasing technique need not

be close to the absorption edge of the anomalous scatterer. A detailed discussion of SAD analysis can be found in Brodersen et al., 2000, Acta Cryst., D56:431-441.

A fifth method of determining phase information is single isomorphous replacement with anomalous scattering or SIRAS. This technique combines isomorphous replacement and anomalous scattering techniques to provide phase information for a crystal of a polypeptide. X-ray diffraction data are collected at a single wavelength, usually from a single heavy-atom derivative crystal. Phase information obtained only from the location of the heavy atoms in a single heavy-atom derivative crystal leads to an ambiguity in the phase angle, which is resolved using anomalous scattering from the heavy atoms. Phase information is therefore extracted from both the location of the heavy atoms and from anomalous scattering of the heavy atoms. A detailed discussion of SIRAS analysis can be found in North, 1965, Acta Cryst. 18:212-216; Matthews, 1966, Acta Cryst. 20:82-86.

Once phase information is obtained, it is combined with the diffraction data to produce an electron density map, an image of the electron clouds that surround the molecules in the unit cell. The higher the resolution of the data, the more distinguishable are the features of the electron density map, e.g., amino acid side chains and the positions of carbonyl oxygen atoms in the peptide backbones, because atoms that are closer together are resolvable. A model of the macromolecule is then built into the electron density map with the aid of a computer, using as a guide all available information, such as the polypeptide sequence and the established rules of molecular structure and stereochemistry. Interpreting the electron density map is a process of finding the chemically reasonable conformation that fits the map precisely.

After a model is generated, a structure is refined. Refinement is the process of minimizing the function Φ , which is the difference between observed and calculated intensity values (measured by an R-factor), and which is a function of the position, temperature factor, and occupancy of each non-hydrogen atom in the model. This usually involves alternate cycles of real space refinement, *i.e.*, calculation of electron density maps and model building, and reciprocal space refinement, *i.e.*, computational attempts to improve the agreement between the original intensity data and intensity data generated from each successive model. Refinement ends when the function Φ converges on a minimum wherein the model fits the electron density map and is stereochemically and conformationally reasonable. During refinement, ordered solvent molecules are added to the structure.

5.9.4.1 Structures of FimCH

5

10

15

20

25

The present invention provides, for the first time, the high-resolution three-dimensional structures and atomic structure coordinates of crystalline FimCH bound to α-D-mannose as determined by X-ray crystallography. The specific methods used to obtain the structure coordinates are provided in the example, *infra*. The atomic structure coordinates of crystalline wild type FimCH - alpha-D-mannopyranoside to 2.8 Å resolution are listed in Table 14. The atomic structure coordinates of crystalline FimCH Q133N - alpha-D-mannopyranoside to 3 Å resolution are listed in Table 15.

5

10

15

20

25

30

35

Those having skill in the art will recognize that atomic structure coordinates as determined by X-ray crystallography are not without error. Thus, it is to be understood that any set of structure coordinates obtained for crystals of FimCH, whether native crystals, heavy-atom derivative crystals or co-crystals, that have a root mean square deviation ("r.m.s.d.") of less than or equal to about 2 Å when superimposed, using backbone atoms (N, $C\alpha$, C and O), on the structure coordinates listed in Table 14 are considered to be identical with the structure coordinates listed in the Table when at least about 50% to 100% of the backbone atoms of FimCH are included in the superposition.

5.9.5 Structure Coordinates

The atomic structure coordinates can be used in molecular modeling and design, as described more fully below. The present invention encompasses the structure coordinates and other information, *e.g.*, amino acid sequence, connectivity tables, vector-based representations, temperature factors, etc., used to generate the three-dimensional structure of the polypeptide for use in the software programs described below and other software programs.

The invention encompasses machine readable media embedded with the three-dimensional structure of the model described herein, or with portions thereof. As used herein, "machine readable medium" refers to any medium that can be read and accessed directly by a computer or scanner. Such media include, but are not limited to: magnetic storage media, such as floppy discs, hard disc storage medium and magnetic tape; optical storage media such as optical discs or CD-ROM; electrical storage media such as RAM or ROM; and hybrids of these categories such as magnetic/optical storage media. Such media further include paper on which is recorded a representation of the atomic structure coordinates, e.g., Cartesian coordinates, that can be read by a scanning device and converted into a three-dimensional structure with an OCR.

A variety of data storage structures are available to a skilled artisan for creating a computer readable medium having recorded thereon the atomic structure

coordinates of the invention or portions thereof and/or X-ray diffraction data. The choice of the data storage structure will generally be based on the means chosen to access the stored information. In addition, a variety of data processor programs and formats can be used to store the sequence and X-ray data information on a computer readable medium. Such formats include, but are not limited to, Protein Data Bank ("PDB") format (Research Collaboratory for Structural Bioinformatics; http://www.rcsb.org/pdb/docs/format/pdbguide2.2/guide2.2_frame.html); Cambridge Crystallographic Data Centre format

5

10

25

30

35

(http://www.ccdc.cam.ac.uk/support/csd_doc/volume3/z323.html); Structure-data ("SD") file format (MDL Information Systems, Inc.; Dalby et al., 1992, J. Chem. Inf. Comp. Sci. 32:244-255), and line-notation, e.g., as used in SMILES (Weininger, 1988, J. Chem. Inf. Comp. Sci. 28:31-36). Methods of converting between various formats read by different computer software will be readily apparent to those of skill in the art, e.g., BABEL (v. 1.06, Walters & Stahl, ©1992, 1993, 1994;

http://www.brunel.ac.uk/departments/chem/babel.htm.). All format representations of the polypeptide coordinates described herein, or portions thereof, are contemplated by the present invention. By providing computer readable medium having stored thereon the atomic coordinates of the invention, one of skill in the art can routinely access the atomic coordinates of the invention, or portions thereof, and related information for use in modeling
 and design programs, described in detail below.

While Cartesian coordinates are important and convenient representations of the three-dimensional structure of a polypeptide, those of skill in the art will readily recognize that other representations of the structure are also useful. Therefore, the three-dimensional structure of a polypeptide, as discussed herein, includes not only the Cartesian coordinate representation, but also all alternative representations of the three-dimensional distribution of atoms. For example, atomic coordinates may be represented as a Z-matrix, wherein a first atom of the protein is chosen, a second atom is placed at a defined distance from the first atom, a third atom is placed at a defined distance from the second atom so that it makes a defined angle with the first atom. Each subsequent atom is placed at a defined distance from a previously placed atom with a specified angle with respect to the third atom, and at a specified torsion angle with respect to a fourth atom. Atomic coordinates may also be represented as a Patterson function, wherein all interatomic vectors are drawn and are then placed with their tails at the origin. This representation is particularly useful for locating heavy atoms in a unit cell. In addition, atomic coordinates may be represented as a series of vectors having magnitude and direction and drawn from a chosen origin to each

atom in the polypeptide structure. Furthermore, the positions of atoms in a threedimensional structure may be represented as fractions of the unit cell (fractional coordinates), or in spherical polar coordinates.

Additional information, such as thermal parameters, which measure the motion of each atom in the structure, chain identifiers, which identify the particular chain of a multi-chain protein in which an atom is located, and connectivity information, which indicates to which atoms a particular atom is bonded, is also useful for representing a three-dimensional molecular structure.

10

15

20

25

30

35

5

5.9.6 Uses of the Atomic Structure Coordinates

Structure information, typically in the form of the atomic structure coordinates, can be used in a variety of computational or computer-based methods to, for example, design, screen for and/or identify compounds that bind the crystallized polypeptide or a portion or fragment thereof, or to intelligently design mutants that have altered biological properties.

In one embodiment, the crystals and structure coordinates obtained therefrom are useful for identifying and/or designing compounds that bind FimC, FimH, FimCH, or a fragment thereof, as an approach towards developing new therapeutic agents. For example, a high resolution X-ray structure will often show the locations of ordered solvent molecules around the protein, and in particular at or near putative binding sites on the protein. This information can then be used to design molecules that bind these sites, the compounds synthesized and tested for binding in biological assays. Travis, 1993, Science 262:1374.

In another embodiment, the structure can be probed with a plurality of molecules to determine their ability to bind to FimC, FimH, FimCH, or a fragment thereof, at various sites. Such compounds can be used as targets or leads in medicinal chemistry efforts to identify, for example, inhibitors of potential therapeutic importance. For example, the structure coordinates can be used to identify compounds that inhibit mannose binding by FimCH. Such compounds can be used, for example, to treat or prevent urinary tract infection by a pathogen expressing FimC, FimH or FimCH.

In yet another embodiment, the structure can be used to computationally screen small molecule data bases for chemical entities or compounds that can bind in whole, or in part, to FimC, FimH, FimCH, or a fragment thereof. In this screening, the quality of fit of such entities or compounds to the binding site may be judged either by shape complementarity or by estimated interaction energy. Meng *et al.*, 1992, J. Comp. Chem. 13:505-524.

- 104 -

The design of compounds that bind to FimC, FimH, FimCH, or a fragment thereof, according to this invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with FimC, FimH, FimCH, or a fragment thereof. This association can be covalent or non-covalent. For example, covalent interactions may be important for designing irreversible inhibitors of a protein. Non-covalent molecular interactions important in the association of FimC, FimH, FimCH, or a fragment thereof, with its substrate include hydrogen bonding, ionic interactions and van der Waals and hydrophobic interactions. Second, the compound must be able to assume a conformation that allows it to associate with FimC, FimH, FimCH, or a fragment thereof. Although certain portions of the compound will not directly participate in this association with FimC, FimH, FimCH, or a fragment thereof, those portions may still influence the overall conformation of the molecule. This, in turn, may have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical group or compound in relation to all or a portion of the binding site, or the spacing between functional groups of a compound comprising several chemical groups that directly interact with FimC, FimH, FimCH, or a fragment thereof].

The potential inhibitory or binding effect of a chemical compound on FimC, FimH, FimCH, or a fragment thereof, may be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques. If the theoretical structure of the given compound suggests insufficient interaction and association between it and FimC, FimH, FimCH, or a fragment thereof, synthesis and testing of the compound is unnecessary. However, if computer modeling indicates a strong interaction, the molecule may then be synthesized and tested for its ability to bind to FimC, FimH, FimCH, or a fragment thereof, and inhibit its activity. In this manner, synthesis of ineffective compounds may be avoided.

25

30

35

20

5

10

15

An inhibitory or other binding compound of FimC, FimH, FimCH, or a fragment thereof, may be computationally evaluated and designed by means of a series of steps in which chemical groups or fragments are screened and selected for their ability to associate with the individual binding pockets or other areas of FimC, FimH, FimCH, or a fragment thereof. One skilled in the art may use one of several methods to screen chemical groups or fragments for their ability to associate with FimC, FimH, FimCH, or a fragment thereof. This process may begin by visual inspection of, for example, the active site on the computer screen based on the coordinates of FimC, FimH, FimCH, or a fragment thereof. Selected fragments or chemical groups may then be positioned in a variety of orientations, or docked, within an individual binding pocket of FimC, FimH, FimCH, or a fragment thereof, as defined supra. Docking may be accomplished using software such as QUANTA and

SYBYL, followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARMM and AMBER.

Specialized computer programs may also assist in the process of selecting fragments or chemical groups. These include:

- 1. GRID (Goodford, 1985, J. Med. Chem. 28:849-857). GRID is available from Oxford University, Oxford, UK;
- 2. MCSS (Miranker & Karplus, 1991, Proteins: Structure, Function and Genetics 11:29-34). MCSS is available from Molecular Simulations, Burlington, MA;

5

25

- AUTODOCK (Goodsell & Olsen, 1990, Proteins: Structure, Function, and
 Genetics 8:195-202). AUTODOCK is available from Scripps Research Institute, La Jolla,
 CA; and
 - 4. DOCK (Kuntz *et al.*, 1982, J. Mol. Biol. 161:269-288). DOCK is available from University of California, San Francisco, CA.

Once suitable chemical groups or fragments have been selected, they can be assembled into a single compound or inhibitor. Assembly may proceed by visual inspection of the relationship of the fragments to each other in the three-dimensional image displayed on a computer screen in relation to the structure coordinates of FimC, FimH, FimCH, or a fragment thereof. This would be followed by manual model building using software such as QUANTA or SYBYL.

Useful programs to aid one of skill in the art in connecting the individual chemical groups or fragments include:

- 1. CAVEAT (Bartlett *et al.*, 1989, 'CAVEAT: A Program to Facilitate the Structure-Derived Design of Biologically Active Molecules'. In Molecular Recognition in Chemical and Biological Problems', Special Pub., Royal Chem. Soc. 78:182-196). CAVEAT is available from the University of California, Berkeley, CA;
- 2. 3D Database systems such as MACCS-3D (MDL Information Systems, San Leandro, Calif.). This area is reviewed in Martin, 1992, J. Med. Chem. 35:2145-2154); and
 - 3. HOOK (available from Molecular Simulations, Burlington, Mass.).
- Instead of proceeding to build an inhibitor of FimC, FimH, FimCH, or a

 fragment thereof, in a step-wise fashion one fragment or chemical group at a time, as
 described above, compounds that bind may be designed as a whole or 'de novo' using either
 an empty active site or optionally including some portion(s) of a known inhibitor(s). These
 methods include:
- 1. LUDI (Bohm, 1992, J. Comp. Aid. Molec. Design 6:61-78). LUDI is available from Molecular Simulations, Inc., San Diego, CA;

2. LEGEND (Nishibata & Itai, 1991, Tetrahedron 47:8985). LEGEND is available from Molecular Simulations, Burlington, Mass.; and

3. LeapFrog (available from Tripos, Inc., St. Louis, Mo.).

5

10

15

20

25

30

35

Other molecular modeling techniques may also be employed in accordance with this invention. *See*, *e.g.*, Cohen *et al.*, 1990, J. Med. Chem. 33:883-894. *See also*, Navia & Murcko, 1992, Current Opinions in Structural Biology 2:202-210.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound may bind to FimC, FimH, FimCH, or a fragment thereof, may be tested and optimized by computational evaluation. For example, a compound that has been designed or selected to function as an inhibitor of FimC, FimH, FimCH, or a fragment thereof, must also preferably occupy a volume not overlapping the volume occupied by the active site residues when the native substrate is bound. An effective inhibitor must preferably demonstrate a relatively small difference in energy between its bound and free states (*i.e.*, it must have a small deformation energy of binding). Thus, the most efficient inhibitors should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mol, preferably, not greater than 7 kcal/mol. Inhibitors may interact with the protein in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the inhibitor binds to the enzyme.

A compound selected or designed for binding to FimC, FimH, FimCH, or a fragment thereof, may be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target protein. Such non-complementary electrostatic interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the inhibitor and the protein when the inhibitor is bound to it preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include: Gaussian 92, revision C (Frisch, Gaussian, Inc., Pittsburgh, PA. ©1992); AMBER, version 4.0 (Kollman, University of California at San Francisco, ©1994); QUANTA/CHARMM (Molecular Simulations, Inc., Burlington, MA, ©1994); and Insight II/Discover (Biosym Technologies Inc., San Diego, CA, ©1994). These programs may be implemented, for instance, using a computer workstation, as are well-known in the art. Other hardware systems and software packages will be known to those skilled in the art.

Once a binding compound has been optimally selected or designed, as described above, substitutions may then be made in some of its atoms or chemical groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, *i.e.*, the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. One of skill in the art will understand that substitutions known in the art to alter conformation should be avoided. Such altered chemical compounds may then be analyzed for efficiency of binding to FimC, FimH, FimCH, or a fragment thereof, by the same computer methods described in detail above.

Because FimC, FimH, FimCH, or a fragment thereof, may crystallize in more than one crystal form, the structure coordinates of FimC, FimH, FimCH, or a fragment thereof,, are particularly useful to solve the structure of those other crystal forms of FimC, FimH, FimCH, or a fragment thereof. They may also be used to solve the structure of mutants, co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of FimC, FimH or FimCH.

15

20

25

10

5

One method that may be employed for this purpose is molecular replacement. In this method, the unknown crystal structure, whether it is another crystal form of FimC, FimH, FimCH, or a fragment thereof, a mutant, or a co-complex, or the crystal of some other protein with significant amino acid sequence homology to any functional domain of FimC, FimH or FimCH, may be determined using phase information from the structure coordinates. This method may provide an accurate three-dimensional structure for the unknown protein in the new crystal more quickly and efficiently than attempting to determine such information ab initio. In addition, in accordance with this invention, mutants may be crystallized in co-complex with known inhibitors. The crystal structures of a series of such complexes may then be solved by molecular replacement and compared with that of wild-type FimC, FimH, FimCH, or a fragment thereof. Potential sites for modification within the various binding sites of the protein may thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between FimC, FimH, FimCH, or a fragment thereof, and a chemical group or compound.

30

35

If an unknown crystal form has the same space group as and similar cell dimensions to the known FimC, FimH or FimCH crystal form, then the phases derived from the known crystal form can be directly applied to the unknown crystal form, and in turn, an electron density map for the unknown crystal form can be calculated. Difference electron density maps can then be used to examine the differences between the unknown crystal form and the known crystal form. A difference electron density map is a subtraction of one

electron density map, e.g., that derived from the known crystal form, from another electron density map, e.g., that derived from the unknown crystal form. Therefore, all similar features of the two electron density maps are eliminated in the subtraction and only the differences between the two structures remain. For example, if the unknown crystal form is of a co-complex, then a difference electron density map between this map and the map derived from the native, uncomplexed crystal will ideally show only the electron density of the ligand. Similarly, if amino acid side chains have different conformations in the two crystal forms, then those differences will be highlighted by peaks (positive electron density) and valleys (negative electron density) in the difference electron density map, making the differences between the two crystal forms easy to detect. However, if the space groups and/or cell dimensions of the two crystal forms are different, then this approach will not work and molecular replacement must be used in order to derive phases for the unknown crystal form.

All of the complexes referred to above may be studied using well-known

X-ray diffraction techniques and may be refined versus 50 Å to 1.5 Å or greater resolution

X-ray data to an R value of about 0.20 or less using computer software, such as CNS (Yale

University, (c) 1992, distributed by Molecular Simulations, Inc.). See, e.g., Blundel et al.,

1976, Protein Crystallography, Academic Press.; Methods in Enzymology, vol. 114 & 115,

Wyckoff et al., eds., Academic Press, 1985. This information may thus be used to optimize

known classes of inhibitors, and more importantly, to design and synthesize novel classes of inhibitors.

The structure coordinates of mutants will also facilitate the identification of related proteins or enzymes analogous to FimC, FimH, FimCH, or a fragment thereof, in function, structure or both, thereby further leading to novel therapeutic modes for treating or preventing FimC, FimH or FimCH, mediated diseases.

Subsets of the atomic structure coordinates can be used in any of the above methods. Particularly useful subsets of the coordinates include, but are not limited to, coordinates of single domains, coordinates of residues lining an active site, coordinates of residues that participate in important protein-protein contacts at an interface, and $C\alpha$ coordinates. For example, the coordinates of one domain of a protein that contains the active site may be used to design inhibitors that bind to that site, even though the protein is fully described by a larger set of atomic coordinates. Therefore, a set of atomic coordinates that define the entire polypeptide chain, although useful for many applications, do not necessarily need to be used for the methods described herein.

35

25

30

5

In carrying out the procedures of the present invention it is of course to be understood that reference to particular buffers, media, reagents, cells, culture conditions and the like are not intended to be limiting, but are to be read so as to include all related materials that one of ordinary skill in the art would recognize as being of interest or value in the particular context in which that discussion is presented. For example, it is often possible to substitute one buffer system or culture medium for another and still achieve similar, if not identical, results. Those of skill in the art will have sufficient knowledge of such systems and methodologies so as to be able, without undue experimentation, to make such substitutions as will optimally serve their purposes in using the methods and procedures disclosed herein.

All publications, patents and patent applications mentioned in this specification are herein incorporated by reference into the specification to the same extent as if each individual publication, patent or patent application was specifically and individually indicated to be incorporated herein by reference.

The present invention will now be further described by way of the following non-limiting examples. In applying the disclosure of these examples, it should be kept clearly in mind that other and different embodiments of the methods disclosed according to the present invention will no doubt suggest themselves to those of skill in the relevant art.

20

25

5

10

15

6. EXAMPLES

6.1 EXAMPLE 1: Characterization of FimH mutants

Based on the crystal structure (Figure 2) of vaccine quality FimCH bound to mono-mannose, the mannose-binding domain on FimH was identified. This domain was in a canyon on the surface of the protein. Furthermore, some of the specific amino acids on FimH mediating the interaction with mannose were identified. A hydrophobic ring around the mannose-binding pocket was also identified. To probe critical structural and conformational requirements of FimH, the crystal structure was used to provide several candidate residues for mutation. The serine at position 62 was mutated to an alanine and used as a control since it does not lay within the pocket or the hydrophobic ring region.

30

6.1.1 Expression and Isolation of FimCH mutants

Site specific mutations in FimH (see Table 7) were made according to techniques known in the art. A two-step PCR protocol as described for the mutagenesis of papD (Hung et al., 1999, Proc. Natl. Acad. Sci. USA 96:8178-83) was used. The following

primers were used to amplify and introduce mutations in the first half of the FimH gene (* = coding strand; # = noncoding strand):

5	EcoRI XcmI	*5'-GGGGGGAATTCACCCGGAGGGATGATTGTA-3' (SEQ ID NO:5) #5'-CCAGTAGGCACCACCACATCATTATTGG-3' (SEQ ID NO:6)
	F1A	*5'-CTGGTCGGTAAATGCCTGGTCAGCGGCCTGTAAAACCGCCAATGGTAC-3' (SEQ ID NO:7)
10		#5'-GTACCATTGGCGGTTTTACAGGCCGCTGACCAGGCATTTACCGACCAG-3' (SEQ ID NO:8)
	I13A	*5'-GCCAATGGTACCGCTATCCCTGCGGGCGGTGGCAGCGCCAATG-3' (SEQ ID NO:9)
15		#5'-CATTGGCGCTGCCACCGCCCGCAGGGATAGCGGTACCATTGGC-3' (SEQ ID NO:10)
	I52A	*5'-CCATAACGATTATCCGGAAACCGCGACAGACTATGTCACACTGC-3' (SEQ ID NO:11)
20		#5'-GCAGTGTGACATAGTCTGTCGCGGTTTCCGGATAATCGTTATGG-3' (SEQ ID NO:12)
	S62A	*5'-GCAACGAGGCGCCGCTTATGGCGG-3' (SEQ ID NO:13)
	N46A	#5'-CCGCCATAAGCGGCGCCTCGTTGC-3' (SEQ ID NO:14)
25	N40A	*5'-CTTTTGCCATGCTGATTATCCGGAAACC-3' (SEQ ID NO:15) #5'-GGTTTCCGGATAATCAGCATGGCAAAAC-3' (SEQ ID NO:16)
	N46D	*5'-CTTTTGCCATGATGATTATCCGGAAACC-3' (SEQ ID NO:17) #5'-GGTTTCCGGATAATCATCATGGCAAAAC-3' (SEQ ID NO:18)
30	Y48A	*5'-GCAAATCTTTTGCCATAACGATGCGCCGGAAACCATTACAGACTATGTCACACTG-3' (SEQ ID NO:19) #5'-CAGTGTGACATAGTCTGTAATGGTTTCCGGCGCATCGTTATGGCAAAAGATTTGC-3'
		(SEQ ID NO:20)

	D54A	*5'-ACCATTACAGCTTATGTCACACTG-3' (SEQ ID NO:21) #5'-CAGTGTGACATAAGCTGTAATGGT-3' (SEQ ID NO:22)
5	D54N	*5'-ACCATTACAAACTATGTCACACTG-3' (SEQ ID NO:23) #5'-CAGTGTGACATAGTTTGTAATGGT-3' (SEQ ID NO:24)
	Q133A	*5'-CTTATTTTGCGCGCTACCAACAAC-3' (SEQ ID NO:25) #5'-GTTGTTGGTAGCGCGCAAAATAAG-3' (SEQ ID NO:26)
10	Q133N	*5'-CTTATTTTGCGAAATACCAACAAC-3' (SEQ ID NO:27) #5'-GTTGTTGGTATTTCGCAAAATAAG-3' (SEQ ID NO:28)
15	Q133K	*5'-CTTATTTTGCGGAAGACCAACAAC-3' (SEQ ID NO:29) #5'-GTTGTTGGTCTTCCGCAAAATAAG-3' (SEQ ID NO:30)
	Q133E	*5'-GCCGTGCTTATTTTGCGAGAAACCAACAACTATAACAGCGATG-3' (SEQ ID NO:31) #5'-CATCGCTGTTATAGTTGTTGGTTTCTCGCAAAATAAGCACGGC-3'
20		(SEQ ID NO:32)
	Q133R	*5'-GCCGTGCTTATTTTGCGACGCACCAACAACTATAACAGCGATG-3' (SEQ ID NO:33) #5'-CATCGCTGTTATAGTTGTTGGTGCGTCGCAAAATAAGCACGGC-3' (SEQ ID NO:34)
25		
_	Q133H	*5'-GCCGTGCTTATTTTGCGACATACCAACAACTATAACAGCGATG-3' (SEQ ID NO:35) #5'-CATCGCTGTTATAGTTGTTGGTATGTCGCAAAATAAGCACGGC-3' (SEQ ID NO:36)
30	N135A	*5'-GCGACAGACGGCCAACTATAACAGC-3' (SEQ ID NO:37) #5'-GCTGTTATAGTTGGCCGTCTGTCGC-3' (SEQ ID NO:38)
35	N135D	*5'-GCGACAGACCGATAACTATAACAGC-3' (SEQ ID NO:39) #5'-GCTGTTATAGTTSTCGGTCTGTCGC-3' (SEQ ID NO:40)

	Y137A	*5'-GCGACAGACCAACACGCGAACAGCGATGATTTCCAGTTTGTG-3' (SEQ ID NO:41) #5'-CACAAACTGGAAATCATCGCTGTTCGCGTTGTTGGTCTGTCGC-3' (SEQ ID NO:42)
5		(62.4.2.1.6.1.2)
	D140A	*5'-CTATAACAGTGCAGATTTCCAG-3' (SEQ ID NO:43)
		#5'-CTGGAAATCTGCACTGTTATAG-3' (SEQ ID NO:44)
	D140N	*5'-CTATAACAGCAATGATTTCCAG-3' (SEQ ID NO:45)
10		#5'-CTGGAAATCATTGCTGTTATAG-3' (SEQ ID NO:46)
	D140E	*5'-CTATAACAGCGAAGACTTCCAG-3' (SEQ ID NO:47)
		#5'-CTGGAAGTCTTCGCTGTTATAG-3' (SEQ ID NO:48)
15	F142A	*5'-GCGACAGACCAACAACTATAACAGCGATGATGCGCAGTTTGTG-3' (SEQ ID NO:49) #5'-CACAAACTGCGCATCATCGCTGTTATAGTTGTTGGTCTGTCGC-3'
		(SEQ ID NO:50)
20		EcoR I and Xcm I restriction sites were engineered into the 5' and 3' primers,
	respectively f	or cloning. The PCR inserts were cloned into an EcoR1 and Xcm1 digested
		generate a full-length FimH gene containing the desired mutations. Mutations
		confirmed by sequencing. Each mutant was subcloned as an EcoR I-BamH I
	•	mH gene into the IPTG-inducible expression vector, pMMB66 (Furste et al.,
25	7	8:119-31). The resulting plasmids, pHACWF1A, pHACWI13A,
	_	A, pHACWI52A, pHACWS62A, pHACWN46A, pHACWN46D,
	_	A, pHACWD54N, pHACWQ133A, pHACWQ133N, pHACWQ133K,
	pHACWQ13	3E, pHACWQ133R, pHACWQ133H, pHACWN135A, pHACWN135D,

encode FimH with point mutations changing Phe-1 to Ala; Ile-13 to Ala; Tyr-48 to Ala; Ile-52 to Ala; Ser-62 to Ala; Asn-46 to Ala or Asp; Asp-54 to Ala or Asn; Gln-133 to Ala, Asn, Lys, Glu, Arg, or His; Asn-135 to Ala or Asp; Tyr-137 to Ala; Asp140 to Ala, Asn, or Glu; and Phe-142 to Ala. Additionally, the FimH gene may be cloned into the pCGA139-1-1 vector (see Section 5.6) for expression. The wild type FimH gene from pHACW18 was also cloned into pMMB66 in the similar manner and designated as pHACW66. The original

pHACWY137A, pHACWD140A, pHACWD140N, pHACWD140E, pHACWF142A

30

PCT/US01/47994 WO 02/102974

pMMB66 expression vector was used as the negative control plasmid for FimH expression. All plasmids were transformed into E. coli strains ORN103/pUT2002, AAEC185/pUT2002, C600/pHJ9205, and K12.

Wild type FimCH is a made up of an ~ 52 kDa complex composed of two wild type proteins; FimC (22.8 kDa) and FimH (29.1 kDa) in a 1:1 equimolar ratio. Periplasmic extracts were isolated as described (Slonim et al, 1992, EMBO J. 11:4747-56 and Jones et al., 1993, Proc. Natl. Acad. Sci. USA 90:8397-8401). Bacterial strain C600/pHJ9205 or K12 transformed with FimH expression constructs was used to produce large quantities of FimH proteins. These transformants were grown in LB in the presence of 10 0.1% arabinose and 0.1 mM IPTG to induce FimC and FimH expression, respectively. The protocol for the purification of FimCH complexes from bacterial periplasm has been described previously and was followed in this study (Barnhart et al., 2000, Proc. Natl. Acad. Sci. USA 97:7709-14, incorporated herein by reference). Purified FimCH complexes were dialyzed into 20 mM MES, pH 6.8 and stored at 4 °C.

Purified recombinant FimH proteins associated with wild type FimC protein. This was assayed by ELISA using an anti-FimC antibody to detect FimCH complexes (Figure 4). Each of the mutant proteins was expressed, associated with FimC, and localized to the periplasm (data not shown).

Table 7: Site Directed Mutagenesis of FimH

5

15

	residue position	wild type amino acid	engineered mutant amino acid
	1	phenylalanine (F)	alanine (A)
	13	isoleucine (I)	alanine (A)
25	46	asparagine (N)	alanine (A)
	46	asparagine (N)	aspartic acid (D)
	48	tyrosine (Y)	alanine (A)
	52	isoleucine (I)	alanine (A)
30	54	aspartic acid (D)	alanine (A)
	54	aspartic acid (D)	asparagine (N)
	62*	serine (S)	alanine (A)
	67	asparagine (N)	alanine (A)
35	67	asparagine (N)	aspartic acid (D)

	75	aspartic acid (D)	alanine (A)
	75	aspartic acid (D)	asparagine (N)
	133	glutamine (Q)	alanine (A)
5	133	glutamine (Q)	lysine (K)
	133	glutamine (Q)	asparagine (N)
	133	glutamine (Q)	histidine (H)
	133	glutamine (Q)	arginine (R)
10	133	glutamine (Q)	glutamic acid (E)
	.135	asparagine (N)	alanine (A)
	135	asparagine (N)	aspartic acid (D)
	135	asparagine (N)	lysine (K)
15	137	tyrosine (Y)	alanine (A)
	140	aspartic acid (D)	alanine (A)
	140	aspartic acid (D)	asparagine (N)
	140	aspartic acid (D)	glutamic acid (E)
20	142	phenylalanine (F)	alanine (A)
	154	glutamic acid (É)	alanine (A)
	154	glutamic acid (E)	asparagine (N)
	154	glutamic acid (E)	lysine (K)
25	156	asparagine (N)	alanine (A)
23	156	asparagine (N)	aspartic acid (D)
	161	aspartic acid (D)	alanine (A)
	161	aspartic acid (D)	asparagine (N)
30	161	aspartic acid (D)	glutamic acid (E)
411	· · · · · · · · · · · · · · · · · · ·	-11 Cd 11 11	

* control reside outside of the mannose-binding pocket and hydrophobic ring regions.

6.1.2 Bacterial Surface Staining of FimH Proteins

Bacterial strain AAEC185/pUT2002 contained a FimH-null type 1 pilus operon and was complemented with either wild type or each of the mutant FimH expression plasmids. These bacteria were cultured in the same manner as the ORN103/pUT2002

transformants for optimal FimH and type 1 pili expression. Overnight cultures were diluted to the same concentration (OD₆₀₀ 1) and 1 ml of diluted bacteria was used to immunostain for FimH on the bacterial surface. Bacterial cultures were washed once in PBS (0.12 M NaCl, 2.7 mM KCl, 10 mM phosphate, pH 7.4) and resuspended in 100 ul PBS+5% FBS containing 1:1000 dilution of anti-FimC/FimH antiserum (MedImmune Inc.). Binding of primary antibody was allowed to proceed for one hour on ice and followed by three washes with PBS. Bacterial pellets were resuspended in 100 ul of Oregon Green-conjugated goatmouse IgG (H+L) secondary antibody diluted 1000-fold in PBS+5% FBS and incubated on ice for another hour. After incubation with secondary antibody, bacteria were washed extensively and fixed with 2% glutaraldehyde (in PBS) with 1 μ g/ml Hoechst stain (Sigma) for 5 min at room temperature (RT). Bacteria were washed once again and resuspended in 100 ul PBS. Five microliters of stained bacteria were spotted on glass microscope slides and allowed to air-dry at room temperature. The staining of FimH on bacterial surfaces was visualized with an Olympus BX60 microscope system.

5

10

15

30

35

WT FimCH as well as all of the mutant FimCH proteins were properly localized to the pilus (although data is not shown, it is summarized in Table 8).

6.1.3 Mannose Binding Properties of mutant FimCH proteins

FimH allelic variants can be broadly divided into two functional groups,

those that bind tri-mannose only and those that also are capable of binding mono-mannose.

Mono-mannose binding activity has been correlated to an increased virulence phenotype amongst uropathogenic *E. coli*. Structural insight into these binding activities was gained by analyzing the effect of each mutation on both mono-mannose and tri-mannose binding.

Mannose binding assays were done with purified FimCH complexes as well as FimCH expressed on in tact *E. coli*.

6.1.3.1 Isolated FimCH Protein

Wild type and mutant FimCH complexes were isolated from *E. coli* and purified. The protein complexes were tested for mannose binding ability through the use of a number of different assays described below. Data is summarized in Table 8.

Hemagglutination Assay

ORN103/pUT2002 E. coli complemented with FimH expression constructs were induced to express FimH and other gene products in the rest of the type 1 operon. Briefly, bacteria were first grown overnight in shaking incubators at 37 °C. On the

following day, bacteria were diluted 10-fold and sub-cultured statically again overnight in the presence of 1 μ M IPTG. Hemagglutination assays with guinea pig erythrocytes were performed following published protocols (Slonim et al, 1992, *EMBO J.* 11:4747-56; Hultgren *et al.*, 1990, *Mol Microbiol.* 4:1311-8 and Duguid *et al.*, 1979, *J. Med. Microbiol.* 12:213). Inhibition of agglutination by a 10 mM solution of α -methyl mannoside was used to demonstrate that the agglutination was dependent on mannose.

WT FimCH, FimCH S62A, and FimCH N46D gave positive results in this assay. All remaining FimCH mutations abolished the ability to agglutinate erythrocytes (*i.e.*, did not bind mannose on the erythrocyte surface).

10

35

5

Binding to Mannose-Coated Sepharose Beads

Sepharose 6B beads were coated with saturating amounts of D-mannose (Sigma) and resuspended in 0.02% Na azide, 15 mM CaCl₂, 1.25 M NaCl, 10 mM Tri-HCl, pH 7.8. Mono-mannose coated beads were washed extensively and resuspended as 50% 15 (v/v) slurry in 20 mM MES, pH 6.8. Twenty micrograms of FimCH complexes and 100 ul of the mono-mannose beads were used in the binding experiments. Proteins and beads were incubated together for 2 hours in a reaction volume of 200 ul. Unbound proteins were removed and beads were washed three times with PBS. The washed beads were divided into 2 equal portions: to one half, 50 ul of SDS-PAGE loading buffer was added for the 20 determination of bound FimCH and 50 ul of 1% methyl-α-D-mannopyranosides were added to the other half in attempt to elute bound FimCH. Elution of bound FimCH complexes were allowed to proceed for 40-60 minutes. Following elution, the supernatants were transferred to fresh tubes and proteins in the bound or eluted fractions were resolved on 15% SDS-PAGE gels. SDS-PAGE was performed following standard laboratory protocols. Gels 25 were stained with Coomassie stain according to standard laboratory procedure to visualize the presence of FimCH.

After Coomassie staining and re-hydration, gels were dried onto cellophane sheets. FimCH bands on gels were scanned as digitized images. The quantitation of FimH-band intensity was performed with NIH Image v. 1.62. The relative amounts of FimH proteins on gels were calculated as the integrated intensity of the area surrounding the FimH band. Same area size was used to calculate the intensity of each FimH band.

WT FimCH, FimCH S62A, FimCH D140A, FimCH D140N, FimCH D140E, FimCH N46A, and FimCH N46D all bound mono-mannose coated beads to approximately the same extent. However, the relative amount of FimCH N46D, FimCH D140A, FimCH D140N, FimCH D140E, and FimCH N46A eluted by D-α-mannopyranoside was two-to

five-fold greater than the amount of wild type WT FimCH or FimCH S62A eluted from the same amount of beads suggesting that these mutations in FimH decreased its affinity for mono-mannose (Figures 5 A-B).

5

10

15

20

35

Mannose Affinity Chromatography

In order to evaluate the binding affinities of FimH mutants, an HPLC-format assay was developed using a commercially available methacrylate resin (PE Biosystems) to which a tri-mannose-BSA conjugate (1-3, 1-6-D mannotriose-BSA) or a mono-mannose-BSA conjugate was coupled via epoxide chemistry. The column, which has a bed volume of 0.2 ml, is equilibrated with Phosphate Buffered Saline (PBS, 33.3 mM phosphate, 150 mM NaCl, pH 7.2) and run at a flow rate of 1 ml/minute. Purified FimCH complexes, containing either wild type or mutant FimH, were used in this assay. Samples were diluted to a concentration between 1 and 10 µg/ml using PBS containing 0.5 % Tween-20 (PBST). The diluted samples were filtered through a microcentrifuge filter (0.45 µM) at 13000 rpm (10,000 x g) for 3 minutes at room temperature. An injected sample of proteins flowed through the column to allow interactions with the tri- or mono-mannose moieties. An injection of 50 ul of sample is followed by a 0.5-minute PBS wash. The bound FimCH is subsequently eluted with 0.1 M H₃PO₄ + 0.15 M NaCl for 2 minutes and detected by intrinsic tryptophan fluorescence, using an excitation wavelength of 280 nm and an emission wavelength of 325 nm. Finally, the column is re-equilibrated with PBS for 2.5 minutes. Affinity measurements relative to the wild type FimH can be determined for the bound FimCH complexes based upon the retention time profile.

FimCH Q133A, FimCH N135A, FimCH D140A, FimCH D140N, FimCH D140E, and FimCH N46A were retained on tri-mannose column similarly to WT FimCH.

However, none of the mutant FimCH protein complexes could bind to mono-mannose coated beads during this assay.

Solid Phase (ELISA) Binding Assay

One characteristic of the FimCH molecule is its ability to bind to mannose and mannose-derivatives through the FimH portion of the molecule. The mannose solid phase binding ELISA assay was developed to measure this binding, and to assess the binding avidity differences of various mutants of FimCH for mannose derivatives. This assay exploits the mannose binding function of the FimH region of the molecule.

Immulon 4 plates were coated overnight at 4°C with 0.1 μg/well of monomannose- or tri-mannose-BSA. On the following day, wells were blocked with 300 ul/well

of PBS+1% BSA+0.02% Sodium azide for 1 hour at 37°C followed by three washes with PBS+0.05% Tween-20 (PBST). FimCH samples were diluted in PBS+0.05% Tween-20+0.1% BSA. One hundred microliters of diluted protein samples were added into each well. Plates were incubated at 37 °C for 1 hour. After incubation with FimCH complexes, wells were washed three times with PBST. Subsequently, biotin-conjugated anti-FimC monoclonal antibody was added to each well and plates were incubated again at 37 °C for 1 hour. At the end of incubation, wells were washed as above and horseradish peroxidase-conjugated streptavidin (1:1000 dilution) (Tropix) was added. Following a 30 minute incubation at 37 °C, wells were washed again as above. ELISA reaction was developed with TMB substrate at room temperature for 10 minutes and stop reaction with 50 ul/well of 2N H₂SO₄. Reaction plates were read on SOFTmax at 450 nm.

5

10

15

20

Wild type FimCH was able to bind tri-mannose approximately 10 times better than mono-mannose as measured by ELISA. A two fold reduction in the relative binding of FimCH N46D to mono-mannose was also detected by ELISA however binding to tri-mannose seemed to be unaffected by the mutation. Binding to mono-mannose in the ELISA by FimCH Q133A, FimCH N135A, FimCH D140A, FimCH D140N, FimCH D140E, and FimCH N46A was undetectable with the exception of FimCH D140N, which showed very low levels of binding. Interestingly, although mutations in residue 140 greatly reduced (FimCH D140N) or abolished (FimCH D140A and FimCH D140E) mono-mannose binding in the ELISA assay, they retained their ability to bind tri-mannose, albeit at reduced levels compared to the wild type protein. (Figures 6 A-B)

6.1.3.2 FimCH Protein Expressed on E. coli

E. coli strain PmmB66 was transfected with cDNA encoding the various

FimH mutants. Because PmmB66 does not endogenously express FimH, all of the FimCH complexes on its surface will contain the FimH mutant protein. Mannose binding ability of the mutant FimCH protein when in the context of a cell surface receptor was examined by the following whole cell solid phase mannose binding assay.

Each well of an Immulon-4 plate (Dynex Technologies, Chantilly, VA) was coated with 2.5 μg/ml of mono-mannose or tri-mannose-BSA (V-labs, Covington, LA) in Carbonate Coating Buffer overnight at 4° C. The wells were aspirated and then blocked with PBS + 1% BSA (300 ml/well) by incubation at 37° C for 1 hour. Plates were then washed three times with PBS + 0.1% Tween + 0.1% BSA. The *E. coli* expressing either wild type or mutant FimCH (8.0x10⁷ CFU/ml) were added to each well and incubated at 37°C for 1 hour, and then washed extensively. Bound bacteria were detected with a 1:400

dilution of a polyclonal anti-E. coli (all antigens)-peroxidase conjugated antibody (BioDesign, Inc., Kennebunk, ME; catalog no. B65004R). After washing three times with PBS + 0.1% Tween + 0.1% BSA, the TMB substrate (100 ml/well) was added and incubated at ambient temperature for optimal time before stopping with 2N $\rm H_2SO_4$. OD₄₅₀ readings were taken to quantify the amount of bacteria bound to the mannose.

FimCH N46D could bind tri-mannose at near wild type levels but had a decrease in its ability to bind mono-mannose (Figure 7E). FimCH S62A could bind mono-and tri-mannose equally well, but at a level that was somewhat decreased from wild type ability (Figure 7H). No significant binding could be detected for FimCH N46A, FimCH D140E, and FimCH Q133K (Figures 7D, 7F, and 7G) on either mono- or tri-mannose. These results are similar to those obtained when testing mannose-binding ability of isolates mutant FimCH proteins (see Section 6.1.3.1).

As a control, plates were coated with the polyclonal anti-*E. coli* antibody and then exposed to *E. coli* expressing the different FimCH mutant proteins. Figure 7I shows that the polyclonal antibody can bind to each of the mutant-expressing *E. coli* equally well. This indicates that any differences in the amount of *E. coli* detected in Figures 7A-H reflect a true difference in mannose binding instead a of a technical difficulty with the detection method.

20

25

30

35

15

5

10

6.1.4 Adherence and Invasion Assays

AAEC185/pUT2002 transformed with FimH expression plasmids were used to assay FimH-mediated bacterial adherence and invasion into the human bladder cell line 5637 (ATCC # HTB-9). Bacteria were cultured as described above for type 1 pili expression. Adherence and invasion assays were performed following published protocols with a minor modification (Elsinghorst & Weitz, 1994, Infect Immun. 62:3463-71; Martinez et al., 2000, EMBO J. 2000 19:2803-12). Instead of a two-hour infection step, bacteria were incubated for one hour to allow for binding and entry into bladder cells.

WT FimCH, FimCH S62A, and FimCH N46D could adhere and invade the bladder cells (although FimCH N46D had a 2-fold decrease in ability when compared to WT FimCH). All of the remaining mutant FimCH proteins, however, had no ability to adhere or to bind bladder cells (Figure 8A). However, all of those *E. coli* expressing a FimCH complex competent to adhere to 5637 cells, could also invade (Figure 8B).

E. coli expressing FimCH proteins were also tested for the ability to bind human bladder tissue sections. AAEC185/pUT2002 transformed with FimH expression plasmids were used to assay FimH-mediated bacterial adherence to tissue sections. Bacteria

were cultured as described above for the optimal expression of type 1 pili. In situ binding to human bladder tissues was performed similarly to previously described protocol with minor modifications (Striker, 1995, Adv Exp Med Biol. 385:141-2; Falk et al., 1993, Proc. Natl. Acad. Sci. USA, 90:2035-2039). Briefly, overnight cultures were diluted to the same concentration (OD₆₀₀ 1) and 1 ml of each diluted bacteria was labeled with fluorescein isothiocyanate (FITC) as described (Falk et al., 1993, Proc. Natl. Acad. Sci. USA, 90:2035-2039). Labeled bacteria were resuspended in 1 ml blocking buffer (PBS+0.25% BSA+0.05% Tween-20). Non-diseased human bladder sections were obtained from the surgical pathology and autopsy files of the Department of Pathology at Washington 10 University and deparaffinized following published protocol Falk et al., 1993, Proc. Natl. Acad. Sci. USA, 90:2035-2039. Human bladder tissues on microscope slides were incubated with 100 ul of freshly FITC-labeled bacteria for 2 hours at room temperature in a humidified chamber. Following bacterial binding, slides were washed extensively with PBS, and fixed for 5 minutes with 2.5% glutaraldehyde in PBS. After fixation, slides were counterstained 15 with 1 µg/ml Hoechst stain for 5 minutes. Upon mounting with cover slips, slides were dried overnight at room temperature in the dark. Visualization of bound bacteria was performed on an Olympus BX60 microscope system.

Both WT FimCH and FimCH S62A mediated a high level of tissue binding in a mannose-inhibitable fashion (Figures 9A-D). Bacteria were seen binding to the luminal surfaces of the bladder sections as well as the sub-layers of the bladder epithelium. FimCH N46D could adhere and invade the bladder cells albeit it had a 2-fold decrease in ability when compared to WT FimCH (Figures 9E-F). Binding mediated by FimCH N46D was inhibited by soluble mannose (Figure 9G). None of the other mutants tested showed significant binding or invasion. (Figures 9H-K). (Data is summarized in Table 8).

25

20

5

30

Table 8

FimH	Pilus	HA				Manne	Mannose Binding				Bladder	Invasion
protein	protein Localization		Affinity Ch	Affinity Chromatography	Ä	Beads	B	ELISA	回	ELISA	Cell	
							(with puri	(with purified FimCH)	with Fim	(with FimCH on E. coli)	Ad	
			Tri-mannose	annose Mono-mannose	Tri- mannose	Mono- mannose	Tri- mannose	Mono- mannose	Tri-mannose	Tri-mannose Mono-mannose		
WT	+	+	+	+	+	+	+(3)	+	+	+	+	+
113A	+	pu	рц	pu	pu		+	+	pu	pu	pu	pu
S62A	+	+	pu	pu	pu	+	pu	pu	(1)+	(2)+	+	+
N46D	+	+	pu	pu	pu	(I)+	+	+(5)	+	-/+	+(5)	+
N46A	+	•	pu	pu	pu	(I) +	pu	1	,		•	
Y48A	+	pu	pu	pu	pu	pu	+	+	pu	pu	pu	pu
152A	+	ри	pu	pu	pu	pu	+	(9) -/+	pu	nd	pu	pu
D54A	+	-	•	,		1	ı	1	pu	pu		
D54N	+	•	,	,	1	1	,	•	pu	pu		
Q133K	+		-		,	1	-	•		1	•	
Q133A	+	٠	+	pu	+	(2)-/+	pu	1	pu	nd	•	
Q133N	+:	,	1	,	,	•	•	_	pu	pu	•	•
Q133E	+	pu	pu	pu	pu	pu	+	(9) -/+	pu	pu	pu	pu
Q133H	+	pu·	pu	pu	pu	pu	1	-	pu	pu	pu	pu
)133R	+	pu	pu	pu	pu	pu	1	•	pu	pu	pu	pu
N135A	+	•	+	pu	+	(2)-/+	pu	1	pu	pu	•	٠
N135D	+	-	-	1		•	1	•	Pi	pu	•	-
Y137A	+	pu	pu	pu	pu	pu	+	(9) -/+	pu	pu	pu	pu
D140E	+	-	+	pu	pu	(1)+	+(4)	•	,	,		1
D140A	+(•	+	pu	pu	+(1)	+(4)	•	pu	pu	•	1
D140N	+	,	+	pu	pu	(1)+	(4)+	-/+	pu	nd		,

nd indicates not determined

WT and mutant protein bind to mono-mannose beads in equal amounts; mutant protein elutes with α-D-mannopyranoside 2-5 fold more easily
 mutant protein binds mono-mannose beads less well than WT protein and elutes with a-D-mannopyranoside 4-5 fold more easily
 WT protein binds tri-mannose 10 fold better than mono-mannose as assayed by ELISA
 mutant proteins bind tri-mannose at reduced levels when compared to WT protein (D140N binds tri-mannose as well as WT binds mono-mannose)
 WT protein binds 2 fold better than mutant protein
 mutant protein binds higher concentration of mono-mannose at 30%-50% WT levels
 mutant protein binds mono- and tri-mannose equally well but decreased from WT levels

6.1.5 Naturally Occurring FimH Mutant

All of the mutations in the mono-mannose binding pocket completely abolished binding to bladder epithelium except for the N46D mutation. The N46D mutation reduced binding to bladder cells by about 50%. It retained the ability to bind tri-mannose with the same relative affinity as wild type FimH but had approximately a 50% reduced affinity for mono-mannose. Thus, mono-mannose but not tri-mannose binding appears to be strictly correlated with the physiologically relevant function of FimH in binding bladder epithelium. Since the amide oxygen that binds O6 is left intact in the N46D mutant, the 50% reduction in mono-mannose and bladder binding is presumably a result of the inability to stabilize the pocket to the same degree as the wild type. Thus, even the slightest change in the mannose binding pocket, in an atom that does not directly bind mannose, still significantly reduces binding, emphasizing why the pocket is invariant amongst 200 uropathogenic isolates (see, e.g., Figure 3).

5

10

15

20

25

30

35

Enterohemorragic E. coli (EHEC) are the cause of hemolytic uremic syndrome which results in acute kidney failure (Noel et al., 1997, Dig. Dis. 15:67-91). This syndrome is thought to be the effect of the Shiga toxin, that enters the blood stream and locates to the kidney due to its receptor binding specificity (Kiyokawa et al., 1998, J. Infect. Dis. 178:178-184; Cooling et al., 1998, Infect. Immun. 66:4355-4366). Although EHEC possess the type 1 pilus gene cluster, there is a lack of an association of EHEC strains with urinary tract infections. Interestingly, an inspection of the FimH gene sequences from three different enterohemorragic strains revealed that the binding pocket residue Asn135 was changed to a lysine (this sequence is depicted in Figure 3 as EC189). A lysine at this position would be predicted to exclude mannose from the binding pocket. A dysfunctional mono-mannose binding pocket would render EHEC unable to colonize the bladder and establish an infection. This may represent a natural selection for a less virulent phenotype since colonization of the urinary tract would lead to a direct delivery of the toxin to the kidney causing drastic and rapid consequences to the host.

6.2 EXAMPLE 2: Production of Antibodies

6.2.1 Polyclonal Antibodies

The immunogenicity of purified FimCH variant proteins were assessed by measuring immunoglobulin G (IgG) titer to FimH T3. FimH T3 is a histidine-tagged fusion protein composed of the first 165 amino acids of the mature (279 amino acids) FimH protein.

C3H/HeJ mice were immunized on day 0 (primary immunization) and booster immunized during week 4 with one of the 7 purified antigens: wild type FimCH (from strain J96), wild type FimCH (vaccine composition), FimCH D140E, FimCH N46D,

FimCH Q133K, FimCH Q133E, and FimCH Q133H. Injections were at doses of 4.0, 1.6, 0.64, and 0.26 µg in MF59 adjuvant (Chiron, Emeryville, CA).

Samples from individual mice treated identically were pooled for serological analysis and diluted 1:100 before serial dilution. Antibody responses were assessed by an ELISA with purified FimH T3 as the capture antigens. The purity of the protein preparations of the capture antigen was 95% pure for FimH T3. In all cases the protein preparations were free of any lipopolysaccharide contaminants. Data for immune responses of such mice to the various FimH adhesins is in Figures 10A-C.

Mice vaccinated with FimCH N46D and FimCH D140E showed comparable response to FimCH T3 by ELISA both at 3 weeks (pre-boost) and at 8 weeks (4 weeks post boost) at all doses when compared to wild type FimCH (Figure 10A and 10B).

Interestingly, mice vaccinated with FimCH Q133K protein induced titers to FimH T3 at 3 weeks (pre-boost) that were approximately 20 fold lower than titers to wild type FimH at all doses. However, titers from the FimCH Q133K immunized mice did increase following the boost at 4 weeks and were now comparable to the wild type protein (Figure 10C). This was true at all doses.

6.2.2 Monoclonal Antibodies

Monoclonal antibodies (MAB) were made directed against purified WT FimCH or FimCH Q133K protein using standard techniques well known in the art. Various proteins were used at a 1 μg/ml concentration as capture antigens in an ELISA assay to determine the epitope of each monoclonal antibody clone. Capture antigens included FimC alone (Table, row 1), wild type and mutant FimCH complexes (Table 9, rows 2-8), and truncated FimH proteins (rows 9-11; T3 is a histidine tagged N-terminal lectin binding domain of FimH from amino acid residues 1-184; T2B is the N-terminal lectin binding domain of FimH from amino acid residues 1-178). FimH specific clones were identified based on positive reactivity with the FimCH or FimCH Q133K complex and a negative reactivity with FimC alone by ELISA (Table 9, compare rows 1-3). Clones 1A7, 1C10, 3E11, and 1F2 bind an epitope on FimH while clones 2B2 and 4G3 bind an epitope on FimC. Interestingly, not all MAB clones that bind to FimH do so equally well. For example, clone 1A7 bound FimCH Q133K better than WT FimCH and did not bind FimCH N135D and FimCH D54A at all (Table 9, rows 2-5) while clone 1C10 bound all FimH-containing complexes equally well (Table 9, rows 2-8).

5

10

15

20

25

Table 9: Binding specificity of monoclonal antibodies

5

10

15

20

35

	1A7	1C10	3E11	1F2	4G3	2B2	positive control
1 - FimC	0.038	0.037	0.039	0.04	0.553	0.697	0.982
2 - FimCH WT	0.328	0.624	0.098	0.845	0.793	1.04	1.1
3 - FimCH Q133K	0.504	0.710	0.318	0.555	0.616	0.900	1.1
4 - FimCH N135D	0.04	0.668	0.038	0.643	0.694	0.951	1.1
5 - FimCH D54A	0.055	0.600	0.042	0.735	0.752	1.02	1.17
6 - FimCH Q133A	0.476	0.734	0.370	0.761	0.734	0.988	1.1
7 - FimCH Q133N	0.351	0.757	0.160	0.700	0.705	0.948	1.1
8 - FimCH D140A	0.093	0.710	0.05	0.828	0.750	1.01	1.15
9 - FimH T3	0.616	0.995	0.204	0.104	0.469	0.047	1.1
10 - FimH T2B Q133K	0.283	1.0	0.180	0.187	0.621	0.046	1.1
11 - FimH T2B WT	0.334	1.04	0.092	0.092	0.116	0.045	1.2

Further information regarding the type of epitope recognized by each MAB clone was obtained by western blot analysis as well as by ELISA under urea-denaturing conditions. Western blotting was carried out according standard laboratory protocols also. Briefly, proteins in SDS-PAGE gels were transferred to PVDF membranes (Schleicher & Schuel) and blocked for one hour in blocking buffer consisting of TBST (500 mM NaCl, 0.05% Tween-20, 20 mM Tri-HCL, pH 7.5)/5% nonfat dry milk/3% bovine serum albumin (BSA). Blots were washed briefly in TBST and incubated with anti-FimC/FimH mouse antiserum diluted 1000-fold in blocking buffer for one hour. Following primary antiserum incubation, blots were washed three times for 5 min each with TBST and incubated for another hour with alkaline phosphatase (AP)-conjugated goat α-mouse IgG (whole molecule) secondary antibody (Sigma) diluted 2000-fold in blocking buffer. Subsequently, blots were washed four times for 5 min each with TBST and once with developer buffer (100 mM NaCl, 5 mM MgCl, 100 mM Tri-HCl, pH 9.5) and then developed with 0.04% NBT+0.02% BCIP (diluted in developer buffer).

The results are summarized in Table 10. Briefly, 1A7 and 1C10 cannot recognize FimCH Q133K protein when the protein is denatured indicating that a conformational epitope is recognized. Alternatively, 1F2 can recognize denatured protein indicating that a linear epitope is recognized.

Table 10: Characterization of MAB against FimCH Q133K

MAB clone	epitope	western blot	ELISA with urea-denatured protein
1A7	bind FimH	no	no
1C10	bind FimH	weak	no
3E11	bind FimH	nd	nd
2B2	bind FimC	nd	nd
1C8	bind FimC	strong	nd
1F2	bind FimH	strong	yes

nd indicates not determined

6.3 EXAMPLE 3: Inhibitory Properties of Polyclonal Antibodies

6.3.1 *in vitro*

Functional inhibitory properties of polyclonal antibodies were measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to guinea pig erythrocytes in a hemagglutination assay and by the ability to inhibit *E. coli* binding to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to transformed human bladder J82 cell line.

20

25

30

35

5

10

15

Hemagglutination Assay

The bacteria were directly labeled with fluorescein isothiocyanate (FITC) and incubated with the antibody to be assayed for 30 minutes at 37°C. The bacteria/antibody mixture was then added to the erythrocytes and allowed to incubate. After multiple washes, mean channel fluorescence was used as an indicator of the amount of FITC-labeled bacteria remaining (and thereby is an indication of the strength of the interaction between the FimCH complex on the *E. coli* and mannose). Lysis II software (Becton Dickinson Immunocytometry Systems) was used for analysis of data.

Figure 11 shows the results from the hemagglutination assay. Increasing dilutions of polyclonal antibodies were used in a set of parallel experiments. Preincubation with polyclonal antibodies raised against FimCH Q133 E, FimCH Q133H, FimCH Q133R, FimCH N135D, and WT FimCH inhibited bacteria binding to the erythrocytes very strongly. Polyclonal antibodies raised against FimCH Q133E and FimCH Q133H were inhibitory at greater dilutions than those used for polyclonal antibodies raised against wild type protein (8-32 times more diluted). Control antiserum from animals that were either not immunized or immunized with MF59 adjuvant alone showed no inhibition.

Inhibition of Binding to Bladder Cells

Functional inhibitory properties of antibodies were measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to transformed human bladder J82 cell line (American Type Culture Collection Accession Number HTB1). The bacteria were directly labeled with fluorescein isothiocyanate (FITC) and incubated with the antibody to be assayed for 30 minutes at 37°C. The bacteria/antibody mixture was then added to 1×10^6 bladder cells at a ratio of 250 bacteria/cell. After multiple washes, samples were assayed by flow cytometry (FACStar PLUS; Becton Dickinson, San Jose, CA) as described in Langermann *et al.* (1997, *Science* 276:607-11; which is hereby incorporated by reference in its entirety). Mean channel fluorescence was used as an indicator of FITC-labeled bacteria bound to the J82 bladder cells. Lysis II software (Becton Dickinson Immunocytometry Systems) was used for analysis of data.

5

15

20

25

30

35

The above functional inhibitory assay was performed using the mutant FimH proteins of the invention. Inhibitory assays were run with the 8 week antisera (4 weeks post boost) from mice vaccinated with FimCH N46D and FimCH D140E and the antisera showed comparable inhibitory titers to the anti-FimH wild type antisera. (Figure 12A and 12B).

Although the absolute titers were low, antibodies to FimCH Q133K had a better *in vitro* functional inhibitory activity when compared to wild type FimH antibodies (Figure 12C). This trend toward superior inhibitory function continued past the 4 week boost. Antisera from mice receiving the 4.0, 1.6, and 0.64 doses of the FimCH Q133K protein was still 100% inhibitory at a 1:1600 dilution. Antisera from mice receiving the 0.26 dose of the mutant protein was still 75% inhibitory at the 1:1600 dilution. This is contrasted with the endpoint inhibitory titer of 1:400-1:800 dilution seen at the highest dose (4.0 μ g) for wild type FimCH protein.

For wild type FimCH and FimCH Q133K, an additional boost at week 18 was given. Inhibitory assays were done with antisera from week 16 and week 20. At week 16 (before the second boost), anti-wild type FimCH antibodies did not inhibit bacteria binding to the bladder cells well (Figure 12D). This is contrasted with anti-FimCH Q133K antibodies. At higher concentrations of antibodies (i.e. 1:50, 1:100, and 1:200 dilutions), the pre-second boost anti-FimCH Q133K still retain inhibitory ability (Figure 12E). At 20 weeks (2 weeks post second boost), the anti-wild type FimCH antibody does regain some inhibitory ability but it is not as dramatic as the anti-FimCH Q133K antibody.

Polyclonal antibodies to WT FimCH can inhibit bacteria binding to uroepithelial cells from diabetic women. Uroepithelial cells were isolated from the urine of

diabetic women. FITC-labeled *E. coli* strain NU14 (expressing WT FimCH) was incubated with polyclonal antibodies to FimC, FimH or FimCH. This decreased bacterial binding to the uroepithelial cells by 65% (data not shown).

6.3.2 *in vivo*

Mice were passively immunized with polyclonal antibodies generated with either WT FimCH or mutant protein (FimCH N135D or FimCH Q133R). Mice were administered 1 mg of polyclonal antibody 4 hours prior to a large bolus challenge live uropathogenic E. coli. Type 1 piliated E. coli strain (NU14) bacteria were collected, washed and re-suspended in phosphate buffered saline (PBS) and cell concentration adjusted to OD = 1.8 (at 600 nm). This bacterial cell suspension was then diluted 1:10 in PBS and used as inoculum. Mice were anaesthetized and then inoculated intraurethrally with 50 ml of E. coli suspension containing about 3 x 10⁷ CFU (colony forming units). CFU determination was done by plating the bacterial suspension on TCA plates and examining cell viability. Two days post-inoculation, the mice were sacrificed and bladders were removed and collected into 500 ml PBS supplemented with 1% mannose. The number of CFUs per bladder was determined by grinding the bladders with a tissue tearer and then plating the suspension on TSA plates after dilution. The mean number of colony forming units per bladder was determined and data was transformed to log CFU/bladder. A decrease in the number of CFUs indicates that the passive immunization had a protective ability. Polyclonal antibodies to both mutant proteins were more protective than those raised against wild type protein (Figure 13). The decrease in CFUs per bladder obtained by administration of polyclonal antibodies raised against mutant FimCH was significant when compared to CFUs per bladder obtained when no antibody was administered as indicated by a T-test (see Table 11).

Table 11: T-test Results

antigen polyclonal antibody raised against	MF 59 alone	no injection
FimCH	0.190	0.581
FimCH N135D	0.00003	0.0043
FimCH Q133R	0.0004	0.080

5

10

15

20

25

6.4 EXAMPLE 4: Inhibitory Properties of Monoclonal Antibodies 6.4.1 in vitro

Functional inhibitory properties of antibodies were measured by the ability to block binding of type 1 piliated bacteria (*E. coli* strain NU14) to guinea pig erythrocytes in a hemagglutination assay and by the ability to inhibit *E. coli* binding to an ELISA plate when trimannose was the capture antigen. Fab fragments were also assayed for inhibitory activity.

5

10

15

20

25

30

35

Hemagglutination Assay

The bacteria were directly labeled with fluorescein isothiocyanate (FITC) and incubated with the antibody to be assayed for 30 minutes at 37°C. The bacteria/antibody mixture was then added to the erythrocytes and allowed to incubate. After multiple washes, mean channel fluorescence was used as an indicator of the amount of FITC-labeled bacteria remaining (and thereby is an indication of the strength of the interaction between the FimCH complex on the *E. coli* and mannose). Lysis II software (Becton Dickinson Immunocytometry Systems) was used for analysis of data.

Figure 14 shows the results from the hemagglutination assay. Increasing dilutions of MAB clone were used in a set of parallel experiments. Preincubation with clone 1A7 inhibited bacteria binding to the erythrocytes very strongly. Clones 1C10 and 3E11 also inhibited bacteria binding when the MABs were supplied in larger quantities. Clones 1F2, 2B2, and 1C8 did not show an inhibitory activity. Figure 15A shows the results of various concentrations of clone 1A7 used in the hemagglutination assay. Figure 15B shows various controls that indicate that this inhibitory activity was due to preincubation with MAB clone 1A7. Guinea pig red blood cells alone do not fluoresce. *E. coli* Nu14 bind to guinea pig red blood cells in the absence of antibody pre-incubation. Pre-incubation of *E. coli* with pre-immune serum does not inhibit binding to guinea pig red blood cells. As expected, pre-incubation with antibodies raised against T3 (a histidine tagged N-terminal lectin binding domain of FimH from amino acid residues 1-184) does inhibit *E. coli* binding to guinea pig red blood cells.

ELISA Binding Assay

Immulon 4 plates were coated overnight at 4 °C with 0.1 μg/well of trimannose-BSA. On the following day, wells were blocked with 300 ul/well of PBS+1% BSA+0.02% Sodium azide for 1 hour at 37 °C followed by three washes with PBS+0.05% Tween-20 (PBST). *E. coli* that had been pre-incubated with the antibody to be assayed (for 30 minutes at 37 °C) was added to the tri-mannose coated well. After incubation, the wells were washed extensively. Optical density at 450 nm (OD₄₅₀) was recorded and used as an indicator

of the amount of bacteria attached to the tri-mannose.

Figure 16 shows the results from the ELISA assay. Pre-incubation of bacteria with either MAB clone 1A7 or 1C10 did inhibit binding to tri-mannose as evidenced by the decrease in OD₄₅₀ with increasing MAB antibody used. MAB clone 1C8 (which recognizes an epitope on FimC) did not demonstrate any inhibitory effect at any amount of MAB used and thus mimicked the negative control data.

Characterization of Fab Fragments

Fab fragments were generated for MAB clones 1A7, 1C10, and 1F2. Fabs were purified before use as potential inhibitors of FimCH-mannose binding in a hemagglutination assay. The assay was done as previously, with results shown in Figure 17. Fab fragments of clone 1A7 inhibited bacteria binding as well as intact MAB clone 1A7. This suggests that clone 1A7 inhibits FimCH binding through a steric hindrance of binding versus agglutination. However, Fab fragments of clone 1C10 displayed a drastic decrease in inhibitory ability when compared with its intact MAB counterpart. This suggests that agglutinating activity is an important part of clone 1C10 MAB's inhibitory activity.

6.4.2 in vivo

Passive immunization protection studies were done with MAB clones 1A7, 1C10, and 1F12. One mg of purified MAB was administered by IP injection to a C3H/HeJ mouse. Four hours after MAB administration, the mouse was challenged intraurethrally with 8.2x10⁷ CFU of uropathogenic *E. coli* NU14. After 48 hours, the animal was sacrificed and the bladder was harvested to determine the resulting CFU per bladder.

Figure 18 shows the results of the passive immunization experiment. MAB clone 1C10 provided significant protection (1.4 log reduction in CFU) against *E. coli* infection. However, neither MAB clone 1A7 or 1F2 showed the ability to protect against the large bolus challenge. The decrease in CFUs per bladder obtained by 1C10 administration was significant when compared to CFUs per bladder obtained when no MAB was administered as indicated by a T-test (see Table 12).

Table 12: T-test Results

MAB clone	no injection
1A7	0.271
1C10	0.002
1F2	0.024

35

30

5

10

15

20

6.5 EXAMPLE 5: Use of Mutant Proteins as Vaccines

The purpose of these studies is to examine the efficacy of FimCH mutant to induce a protective immune response in primates.

5

10

15

20

25

30

35

6.5.1 Monkey Vaccination

A recombinant FimC and a mutant FimH complex is purified to over 99% purity from the periplasm of *E. coli* K12 strain 600 as described in Jones *et al.* (1993, *Proc. Natl. Acad. Sci. USA* 90:8397-401).

Bacteria is cultivated in LB agar. Expression of type 1 pili is induced by two 48 hour passages in static brain-heart infusion broth (Difco Labs, Detroit) culture at 37°C. Before infection, expression of type1 pili is quantitated by titration of bacterial suspension and mixing of equal volumes of 3% yeast cells and bacteria in microtiter cells to assay agglutination titers (titers equal to or over 30-60 indicate type 1 pili expression). After bacterial challenge in the monkeys, urine samples from days 2, 4, 7 and 12 after challenge are counted by streaking 100 L of serial 10 step dilution onto cystine-lactose-electrolyte deficient agar plates by means of sterile plastic disposable loops. After incubation overnight at 37°C, E. coli colonies are counted to establish the number of CFU/ml in the urine. A urine specimen is considered positive when it contains at least 100 CFU/ml. To establish that inoculating strain was recovered in urine, urinary bacteria are biochemically analyzed on prepared microplates for rapid typing of coli form bacteria using PhenePlate systems.

The surfactant stabilized emulsion adjuvant MF59 is used to emulsify the mutant FimCH complex and for adjuvant administration. Cynomolgus monkeys receive either 100 µg of mutant FimCH in MF59 adjuvant at a 1:1 ratio, or MF59 plus diluent at weeks 0, 4, and 48. Each 1 ml injection is administered intramuscularly in the thigh (legs are alternated for each injection). Serum samples are collected once a month after vaccination for assessment of immune responses.

Vaginal wash and serum samples are also collected before and after the last boost (weeks 47 and 50). The vaginal wash samples are diluted 1:2 in 0.5% bovine serum albumin, 0.5% milk and 0.2% azide before analysis. Antibody levels are recorded as actual OD at 405 nm (values <2x background were considered negative).

In addition, functional assays are performed with the serum and vaginal washes to demonstrate the efficacy of the vaccine to induce an anti-FimH immunoglobulin response.

With respect to the serum samples, type 1 piliated NU14 *E. coli* are directly labeled with fluorescein isothiocyanate and incubated with 10⁶ J82 bladder cells at a ratio of

250 bacteria/cell in the presence of preimmune or immunized serum and incubated for 30 minutes at 37°C. After multiple washes, samples are assayed by flow cytometry, and percent inhibition is determined relative to preimmune samples from each monkey.

Vaginal washes are also tested to determine if the titer of antibodies in the washes of vaccinated subjects are sufficient to inhibit *E. coli* binding to trimannose. Briefly, 2.5 μg/ml of trimannose-bovine serum albumin is coated on Immulon-4 plates (Dynex Technologies, Chantilly, VA). Type 1 piliated NU14 bacteria (8.0 x 10⁷ CFU/ml) is added to each well, incubated at 37°C for one hour, washed extensively and bound bacteria are detected with 1:400 dilution of anti-*E. coli* horseradish peroxidase conjugated antibody (BioDesign, Kennebunk, ME). Percent inhibition is assessed as a ratio, where % inhibition = [(full signal values - sample value)/full signal value] x 100.

All test monkeys are infected 18 days after the final immunization with *E. coli*. Bladder infection is induced by inoculation of bacterial suspension (1 ml, 10⁸ CFU/ml) via urethral catheter. Urine samples are obtained on days 2, 4, 7, 12 and 14 after challenge to determine the number of bacteria per milliliter of urine, as a measure of infection. Urine samples are also tested for leukocytes as an indicator of inflammation.

Normal flora is also tested to determine whether systemic vaccination with the mutant FimCH adhesin polypeptide affects the normal intestinal flora. *E. coli* recovered from fecal suspensions from each monkey is tested in the PhP assay. All monkeys in both vaccine groups showed normal coliform bacterial growth.

6.5.2 Human Vaccination

Recombinant highly purified mutant FimCH is formulated in the squalene-based adjuvant MF59C.1 to examine safety and immunogenicity in a randomized, controlled, double blind Phase I clinical trial in healthy adult women who are seronegative for anti-FimH antibodies.

Methods

5

10

15

20

25

30

35

The soluble 52 kDa recombinant protein complex of FimC and mutant FimH, FimCH, is recovered from lysed bacteria using a three step chromatographic process. The bulk product is sterile filtered and vialed in a citrate buffer. Shortly before injection into a subject, the FimCH composition is mixed with a squalene-based emulsion adjuvant known as MF59C.1 (Chiron Corp., CA).

In vitro binding to human tissues, purified receptors or receptor homologues is often used to elucidate the roles in virulence of many different adhesins, including pilus-associated adhesins. Similarly, assaying for the ability of such antibodies to block

attachment of bacteria to cells or specific receptors can assess the functionality of antibodies to adhesins. This allows for rapid *in vitro* assessment of serological cross-reactivity between antibodies raised to a single adhesin, such as FimCH purified from one strain of *E. coli*, against a wide range of *E. coli* clinical isolates expressing highly homologous, yet phenotypically distinct FimH adhesins.

The ability of the anti-FimH adhesin antibodies to block bacterial binding to bladder epithelial cells is investigated *in vitro* using a flow cytometric method originally developed for evaluating Rickettsia-cell attachment (Li and Walker, 1992, Infect Immun. 60:2030-5, which is incorporated herein in its entirety).

5

10

15

20

25

30

35

The bacterial binding inhibition assay is run as follows. Type 1-piliated *E. coli* (cystitis, pyelonephritis, gut etc.) isolates are directly labeled with FITC and incubated with 2x10⁶ J82 bladder cells, at a ratio of 250 bacteria/cell, in the presence of pre-immune or hyper-immune serum (murine, rabbit, primate or human antisera) and allowed to mix with the bacteria for 30 minutes at 37°C. Antisera are added at dilutions typically ranging from 1:50 to 1:6400 (two-fold serial dilutions). After multiple washes, samples are assayed by flow cytometry in a FACStar PLUS (Becton Dickinson) according to previously published methods (Langermann *et al.*, 1997, *Science*, 276:607-11). Mean channel fluorescence is used as an indicator of FITC-labeled bacteria bound to J82 bladder cells.

Endpoint inhibitory titers are defined as the titer, after serial two fold dilutions, at which the MCF value (representing bacteria bound to cells) is less than or equal to 50% of the MCF value for the control samples (where control is bacteria incubated with pre-immune serum). To confirm binding and inhibition, J82 bladder cells can be sorted from the flow cytometric adherence assay described and analyzed by fluorescent microscopy and the number of fluorescent bacteria attached to 40 bladder cells visually quantitated.

This assay can be run with vaginal wash samples as long as the samples are collected by straight lavage ("PBS washes"). For vaginal wash samples, inhibitory titer ratios are measured for all samples at a 1:2 dilution. Inhibition cannot be run with vaginal antibody samples collected by the cel-wec method, as this method relies upon a detergent-based extraction buffer which interferes with the binding assay.

Functional inhibitory antibodies to FimCH are also evaluated in an assay called the $E.\ coli$ trimannose-binding assay. Briefly, Immulon-4 plates (Dynex Technologies, Inc., Chantilly, VA) are coated with 2.5 µg/ml (100 ml/well) of tri-mannose-BSA (V-Labs, Covington, LA). Type 1-piliated NU14 (8.0 x 10^7 CFU/ml) are added to each well, incubated at 37°C for 1 hour and after extensive washing, bound bacteria are detected with a 1:400 dilution of an anti- $E.\ coli$ -HRP conjugated antibody (BioDesign, Kennebunk, ME). OD₄₅₀ readings of these samples establish the full signal values (FSV) for binding to trimannose

(approximately 2.0). Additional samples are run in the presence of 1:50 dilutions of serum to assess inhibition, where percent inhibition equals the FSV - the sample value/FSV \times 100. All samples are run in triplicate.

Antibody sampling of vaginal secretions from primates was performed with a sterile cotton swab. The swab was then suspended in 1 ml of PBS, yielding the solution to test for antibodies. The samples were centrifuged at 2,000 X g for 10 minutes at 4°C. The supernatant was treated with Nonidet P-40, aliquoted and stored at -70°C. Antibody sampling of cervical secretions from humans was performed using an absorbent sponge called a Cel-Wec. Cervical secretions (Immunoglobulin) were eluted from sponges "Weck-Cel Spears" with elution buffer: 1 x PBS, 0.5% IGEPAL® (nonionic detergent), Protease inhibitors (1 mg/ml Aprotinin, 1 mM Leupeptin, Bestatin). Antibody sampling of urine samples was done on straight, undiluted urine samples from "clean catch" specimens.

Quantitation of Human IgG in Serum/Urine/Cervical Secretion Samples ELISA Procedure

96 well ELISA plates are coated with capture antibody:

mouse anti human IgG (1 µg/ml CO3 buffer)

Standard*: Human IgG whole molecule (1000 ng-977 pg/ml)

Samples: Human urine or cervical secretions in PBS (diluted two fold 1:2 to 1:64)

Secondary: Biotin labeled goat F(ab'2) anti-human IgG

Tertiary: streptavidin Horse Radish Peroxidase

Substrate: TMB

5

10

15

20

25

30

35

Plates are read at 450nm and quantity determined by SOFTmax software

* to generate a standard curve this is run along with the urine, cervical secretion samples

In order to determine IgG quantity, each urine and cervical secretion sample is run in duplicate at six different dilutions (for all individuals tested). The quantity for each dilution is automatically calculated by SOFTmax using a 4 parameter standard curve (range 1000 ng-977 pg/ml). Only the quantities derived from OD values that fall within the linear range of the standard curve are used to determine the amount of IgG in a serum sample. These quantities are averaged to determine amount of IgG in a sample.

Clinical Procedures

Four cohorts of 12 subjects are randomized at a ratio of 3:1 (*i.e.*, four groups where nine subjects receive the vaccine and 3 subjects receive the adjuvant alone) and, in a sequential fashion, given intramuscular doses of vaccine or control. Mutant FimCH is prepared for injection into a subject immediately prior to the injection, *i.e.*, mixed with diluent and adjuvant. Doses of either 1, 5, 25 or 123 µg of mutant FimCH in 0.5 ml of MF59C.1, or

the control (MF59C.1 alone) are injected slowly, *i.e.*, 20 to 30 seconds, into the deltoid muscle of the upper arm of the subjects at day 0, followed by a booster dose at about 28 days followed by a second booster dose at about 180 days.

To test if the mutant FimCH vaccine is immunogenic in the human subjects, evidence of a clear dose response is looked for. Serum, urine, and vaginal secretions of vaccine recipients is used in Western blot and ELISA assays to determine levels of anti-mutant FimH antibodies. Also, immune serum from vaccine recipients is assayed for inhibitory activity by addition to uropathogenic *E. coli* before exposure to J82 human uroepithelial cell line (bladder cells) *in vitro*. Inhibition of binding of *E. coli* to J82 cells indicates the presence of inhibitory antibodies.

5

10

15

20

25

30

35

6.6 EXAMPLE 6: Preparation Of Co-Crystals Of <u>FimCH and α-D-Mannopyranoside</u>

The subsections below describe the production of the FimCH complex and the preparation and characterization of diffraction quality co-crystals of FimCH with α-D-mannopyranoside.

6.6.1 Production and Purification of FimCH

Plasmid pHACW18 was constructed by cloning fimH into the EcoR I and BamH I sites of pUC18 (Norrander et al., 1983 Gene 26:101-6). Briefly, the fimH gene was amplified from pHJ20 (Jones et al., 1995 Proc Natl Acad Sci USA. 92:2081-5) by polymerase chain reaction (PCR) using Vent Polymerase (New England Biolabs). The resulting fimH gene was confirmed by sequencing. Plasmid pHJ9205 contained the fimC open reading frame driven by the inducible arabinose promoter and was used for the co-expression of FimH proteins. The plasmid pUT2002 having a fimH deleted type 1 operon driven by the natural promoter was described previously (Minion et al., 1989, J Bacteriol 165:1033-6).

The *E. coli* strain C600 (Sambrook *et al.*, *Molecular Cloning: A Laboratory Manual*, 2nd ed., Cold Spring Harbor Laboratory Press, New York (1989)) was used in this study. All bacteria used were grown in Luria Broth (LB) with appropriate antibiotics. Periplasmic extracts were isolated as described (Slonim *et al.*, 1992, *EMBO J.* 11:4747-56). Bacterial strain C600/pHJ9205 transformed with FimH expression constructs was used to produce large quantities of FimH proteins. These transformants were grown in LB in the presence of 0.1% arabinose and 0.1 mM IPTG to induce FimC and FimH expression, respectively. The protocol for the purification of FimCH complexes from bacterial periplasm has been described previously and was followed in this study (Barnhart *et al.*, 2000, *Proc. Natl. Acad. Sci. USA* 97:7670-2), which is hereby incorporated by reference in its entirety. Purified FimCH

complexes were dialyzed into 20 mM MES, pH 6.8 and stored at 4 °C.

5

10

15

20

25

30

35

6.6.2 Preparation Of FimCH - α-D-Mannopyranoside Co-Crystals

The FimCH complex was co-crystallized with α -D-mannopyranoside by vapor diffusion in 4 ml hanging drops. 2 ml of FimCH at OD 5.9 (4.7 mg/ml) in 20 mM MES pH 6.5 and 7 mM α -D-mannose was mixed with 2 ml of 1.0 M (NH₄)₂SO₄ and 100 mM TRIS-HCl pH 8.2 and equilibrated against the latter solution. After 1 week the drops were streak seeded from drops containing small crystalline FimCH. Single bipyramidal crystals about 0.4 mm large in each dimension were fully grown after 2 weeks. The crystals were frozen in after sequentially washing in 1.2 M (NH₄)₂SO₄, 100 mM Tris pH 8.2 complemented up to a final 25 % glycerol in steps of 5% glycerol.

6.6.3 Analysis And Characterization Of FimCH - α-D-Mannopyranoside Co-Crystals

Diffraction Data Collection

Diffraction data sets were collected at beamline 19BM at Advanced Photon Source, Argonne, USA. Processing of the data was performed with an HKL2000 (Otwinowski & Minor,1997, *Methods in Enzymology* 276:307-326). The crystals were frozen after sequentially soaking in 5% up to a final 25 % glycerol in 1.2 M (NH₄)₂SO₄ and 100 mM Tris pH 8.2. The space group was C2 with strong pseudotetragonal features. Unit cell dimensions were a=138.077, b=138.130, c=215.352, b=90.005 for FimCH mannose.

Structure Determination

Rigid body refinement was performed using the FimCH structure (PDB entry code 1QUN) as the model. The refinement was started using a high temperature (3500 K) slowcool stage to remove model bias. Subsequent positional and individual B-factor refinements were performed without s cut-off, using CNS (Brunger et al., 1998, Acta Crystallogr D Biol Crystallogr. 54:905-21). At this stage, electron densities were inspected and four of the eight molecules in the asymmetric unit were found to have good electron density, in contrast with their four non-crystallographically related partners that had a significant part of the pilin domain of the adhesin and the chaperon disordered. The electron density of the receptor binding domain of the adhesin of all eight of the FimCH molecules was clearly defined and showed a mannoside in the carbohydrate binding pocket. Refinement and model building led to final $R_{\rm free}$ and R factors of 0.279 and 0.239 (50 – 2.8 Å) for FimCH mannose.

Structure Analyses

Table 13 summarizes the X-ray crystallography refinement parameters of the structure of the crystalline FimCH - α -D-mannopyranoside co-complex of the invention.

5			le 13 Refinement Summary
	space group		<u>C2</u>
	unit cell	a (Å)	138.077
		<u>b (Å)</u>	<u>138.130</u>
		<u>c (Å)</u>	<u>215.352</u>
10	•	<u>b (°)</u>	90.005
10	Molecules per asymmet	<u>tric unit</u>	<u>8</u>
	Resolution		50.0 - 2.8
	number of observed ref	<u>lections</u>	<u>370.427</u>
	number of unique reflec	ctions	· <u>99.138</u>
	highest resolution shell		<u>2.9-2.8</u>
	R-merge (%)		<u>6.9 (47.8)</u>
15	completeness (%)		<u>99.8 (99.9)</u>
13	$\leq I/s(I) \geq$		13 (2.7)
	reflections with $I > 2$	•	83.8 (52.4)
	Number of protein aton	<u>1S</u>	<u>29.168</u>
	Number of water molec	<u>ules</u>	<u>636</u>
	sigma cut-off used in re	finement	None
	crystallographic R-facto	<u>or</u>	0.239 (0.35)
20	R _{free}		0.279 (0.42)
	r.m.s. bond lengths (Å)		0.007
	r.m.s. bond angles (deg.	Ĵ	<u>1.4</u>

25

30

Table 14 provides the atomic structure coordinates of the crystalline FimCH - α -D-mannopyranoside co-complex in Protein Database Format. The amino acid residue numbers coincide with those used in Figure 2.

Structures coordinates for the crystalline FimCH -\alpha-D-mannopyranoside co-complex according to Table 13 may be modified by mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of the raw structure coordinates and any combination of the above.

6.6.4 Mutant FimCH - α-D-Mannopyranoside Co-Crystals

The structure of the FimCH complex containing the Q133N mutation, derived from crystals grown in the presence of methyl-α-D-mannopyranoside, shows binding of the receptor (Figure 19B). The electron density is strongest at positions C4, C5 and C6 of the - 137 -

sugar. The α-linked methyl group on the anomeric O1 of mannose points outwards away from the pocket and makes a hydrophobic contact with Tyr48 (at 3.7 Å). Asn133 does not link to O3 of the mannose. Interestingly, the Q133N mutation not only affects the interactions originally made by Gln133, but the mannose also loses interaction with Asp140 and Asn135 (Figure 19). The mannose has shifted 0.7 Å from its position in the wild type. A shift in the protein backbone at Asp140 of about 0.7 Å together with changes in the side chain conformations of the Asn133, Asn135, Asn138 and Asp140 enables these residues to take part in a very different hydrogen bonding network (Figure 19B) than was present in the wild type FimCH-mannose structure (Figure 19A). This new hydrogen bonding network includes a new water molecule, W2, that interacts directly with O3. In contrast, the O2 ligand residues remained conserved including W1. W1 interacts both with O2 and the amide group of amino acid 133, as in the wild type complex. The hydrophobic part of the Gln133 side chain makes close van der Waals contacts with the Phe1 aromatic ring (Figure 19A). The shorter Asn133 side chain compensates for the lack of the penultimate carbon Cy of Gln133 by establishing an amino-aromatic stacking interaction: Asn133 points its amide nitrogen atom towards the Phe1 ring (Figure 19B). Phe1 further stacks with Phe144. These stacking interactions in the βstrands holding the loop between Gln133 and Phe142 support the bottom part of the binding site formed by Asn46, Asp47 and Asp54. These results therefore explain how mutating a side chain can dramatically affect the structure of the mannose binding pocket.

20

5

10

15

25

30

			<u>le 15</u>
		Data Collection and	Refinement Summary
	space group		<u>C2</u>
	unit cell	<u>a (Å)</u>	<u>138.349</u>
		<u>b (Å)</u>	<u>138.334</u>
5	•	<u>c (Å)</u>	<u>213.212</u>
J		<u>b (°)</u>	<u>89.983</u>
	Molecules per asymm	etric unit	8
	Resolution	•	<u>45-3.0</u>
	number of observed re	eflections	197,848
	number of unique refle	ections	72,289
	highest resolution shel	1.	3.11-3.0
10	R-merge (%)		8.7 (51.0)
	completeness (%)		87.1 (65.9)
	$\leq I/s(I) \geq$		10.6
	reflections with $I > 2$		82.3 (60.8)
	Number of protein ato	<u>ms</u>	29,160
	Number of water mole	cules	377
	sigma cut-off used in r	efinement	None
15	crystallographic R-fact	tor	0.236 (0.36)
	$\underline{R}_{\text{free}}$		0.280 (0.39)
	r.m.s. bond lengths (Å)	0.007
	r.m.s. bond angles (des	g.)	1.3

Table 16 provides the atomic structure coordinates of the crystalline FimCH

20 Q133N - α-D-mannopyranoside co-complex in Protein Database Format. The amino acid residue numbers coincide with those used in Figure 19.

Structures coordinates for the crystalline FimCH $-\alpha$ -D-mannopyranoside cocomplex according to Table 15 may be modified by mathematical manipulation. Such manipulations include, but are not limited to, crystallographic permutations of the raw structure coordinates, fractionalization of the raw structure coordinates, integer additions or subtractions to sets of the raw structure coordinates, inversion of the raw structure coordinates and any combination of the above.

Equivalents

Those skilled in the art will recognize, or be able to ascertain using no more than routine experimentation, many equivalents to the specific embodiments of the invention described herein. Such equivalents are intended to be encompassed by the following claims. without undue experimentation, to make such substitutions as will optimally serve their purposes in using the methods and procedures disclosed herein.

Table 14

```
REMARK coordinates from minimization and B-factor refinement
REMARK refinement resolution: 45.0 - 2.79 A
REMARK starting r= 0.2400 free_r= 0.2781
REMARK final
                   r= 0.2393 free r= 0.2788
REMARK rmsd bonds= 0.007084 rmsd angles= 1.39839
REMARK B rmsd for bonded mainchain atoms= 2.296 target= 2.0
REMARK B rmsd for bonded sidechain atoms= 3.458 target= 3.5
REMARK B rmsd for angle mainchain atoms= 3.912 target= 3.5
REMARK B rmsd for angle sidechain atoms= 4.836 target= 4.0
REMARK target= mlf final wa= 4.53034
REMARK final rweight= 0.0917 (with wa= 4.53034)
REMARK cycles= 2 coordinate steps= 30 B-factor steps= 30
REMARK sg= C2 a= 138.077 b= 138.130 c= 215.352 alpha= 90.000 beta= 90.005 gamma=
REMARK topology file 1 : CNS_TOPPAR:protein.top
REMARK topology file 2 : CNS TOPPAR:dna-rna.top
REMARK topology file 3 : CNS_TOPPAR:water.top
REMARK topology file 4 : CNS_TOPPAR:ion.top
REMARK topology file 5 : CNS_TOPPAR:carbohydrate.top
REMARK parameter file 1 : CNS_TOPPAR:protein_rep.param
REMARK parameter file 2 : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 3 : CNS_TOPPAR:dna-rna_rep.param
REMARK parameter file 4 : CNS_TOPPAR:dop-raperam
REMARK parameter file 4 : CNS_TOPPAR:ion.param
REMARK parameter file 5 : CNS_TOPPAR:carbohydrate.param
REMARK molecular structure file: water pick6.mtf
REMARK input coordinates: refl4water6.pdb
REMARK reflection file= chwt35dman batch2 C2.cv
REMARK ncs= restrain ncs file= ncs.def
REMARK B-correction resolution: 8.0 - 2.79
REMARK initial B-factor correction applied to fobs :
           B11= 1.259 B22= 2.899 B33= -4.158
B12= 0.000 B13= 0.000 B23= 0.000
REMARK
REMARK
REMARK B-factor correction applied to coordinate array B:
                                                                                  1.274
REMARK bulk solvent: density level= 0.319338 e/A^3, B-factor= 66.2774 A^2
REMARK reflections with | Fobs | /sigma_F < 0.0 rejected REMARK reflections with | Fobs | > 10000 * rms(Fobs) rejected REMARK theoretical total number of refl. in resol. range:
                                                                                   100483 ( 100.0 % )
REMARK number of unobserved reflections (no entry or |\bar{F}|=0):
                                                                                     1348 (
                                                                                                1.3 % )
REMARK number of reflections rejected:
                                                                                        0 (
                                                                                                0.0 %)
REMARK total number of reflections used:
                                                                                    99135 (
                                                                                               98.7 % )
REMARK number of reflections in working set:
                                                                                    89199 (
                                                                                                88.8 % )
REMARK number of reflections in test set:
CRYST1 138.077 138.130 215.352 90.00 90.00 90.00 C 2
                                                                                     9936 (
                                                                                                 9.9 %)
REMARK FILENAME="refine15_mlf.pdb"
REMARK DATE:04-May-01 07:53:09
                                                   created by user:
REMARK VERSION: 1.0
             1 C GLY A
2 O GLY A
3 N GLY A
MOTA
                                 1
                                           44.573 13.325 36.795 1.00 50.79
                                           45.727 13.137 36.430 1.00 53.80
44.144 15.634 37.392 1.00 51.83
43.847 14.586 36.389 1.00 51.84
MOTA
                                  1
MOTA
                                  1
             4 CA GLY A
MOTA
                                  1
                                           43.915 12.471 37.571 1.00 45.13
MOTA
             5 N
                       VAL A
                                  2
             6 CA VAL A
MOTA
                                  2
                                           44.533 11.231 38.004 1.00 37.93
MOTA
             7 · CB VAL A 2
                                          44.363 11.029 39.510 1.00 36.03
                                                                                                 A
                                2
                                           44.840 9.652 39.889 1.00 41.26
45.155 12.087 40.273 1.00 30.35
MOTA
             8 CG1 VAL A
                                                                                                 Α
                 CG2 VAL A
ATOM
```

						•				رة
ATOM	10	C		LА		43.883	10.081	37.256	1.00 38.28	A
ATOM	11	0		L A		42.659	9.966	37.238	1.00 40.70	A
ATOM	12	N		A A		44.699	9.234	36.625		A
ATOM	13	CA		A A		44.162	8.111	35.852	1.00 34.00	A
ATOM	14	CB		A A		44.263	8.408	34.383	1.00 29.35	A
ATOM	15	C		A A		44.781	6.763	36.132	1.00 31.29	A
MOTA	16	0		A A		45.969	6.652	36.389	1.00 35.76	A
ATOM	17	N		JΑ	_	43.948	5.735	36.092	1.00 30.26	A
ATOM	18	CA		JA		44.409	4.381	36.310	1.00 30.36	A
ATOM	19	CB	LEU		4	43.248	3.485	36.724	1.00 30.63	A
ATOM	20	CG	LEC		4	42.519	3.868	38.004	1.00 26.03	A
ATOM	21		. LE		4	41.555	2.748	38.400	1.00 22.68	A
ATOM	22		LEC		4	43.528	4.116	39.087	1.00 24.80	A
ATOM	23	C	LEU		4	44.983	3.882	34.992	1.00 32.66	A
ATOM	24	0	LEU		4	44.537	4.318	33.915	1.00 31.47	A
MOTA	25	N	GL7		5	45.954	2.967	35.088	1.00 31.82	A
ATOM	26	CA	GL7		5	46.607	2.400	33.915	1.00 26.34	A
ATOM ATOM	27	C	GLY		5	45.895	1.217	33.286	1.00 29.91	A
ATOM	28	0	GLY		. 5	46.403	0.617	32.351	1.00 37.42	A
ATOM	29 30	N	ALA		6	44.723	0.864	33.792	1.00 30.92	A
. ATOM	31	CA	ALA		6	43.953	-0.243	33.228	1.00 32.99	A
ATOM	32	CB C	ALA ALA		6	44.337	-1.545	33.895	1.00 28.43	A
ATOM	33	Ö	ALA		6	42.479	0.041	33.465	1.00 33.61	A
ATOM	34	И	THR		6	42.138	0.818	34.348	1.00 42.05	A
ATOM	35	CA	THR		7 7	41.606	-0.584	32.694	1.00 28.40	A
ATOM	36	CB	THR		7	40.184	-0.367	32.860	1.00 24.73	A
ATOM	37	OG1			7	39.478	-0.133	31.503	1.00 21.10	A
ATOM	38	CG2		–	7	39.490 40.168	-1.335	30.716	1.00 14.28	A
ATOM	39	C	THR		7	39.578	1.004 -1.573	30.737	1.00 19.37	A
ATOM	40	ō	THR		7	38.359	-1.722	33.538	1.00 29.26	A
ATOM	41	N	ARG		8	40.447	-2.443	33.598 34.035	1.00 30.92	A
ATOM	42	CA	ARG		8	40.026	-3.654	34.739	1.00 30.29	A
ATOM	43	CB	ARG		8	39.248	-4.596	33.823	1.00 30.40	A
ATOM	44	CG	ARG		8	40.131	-5.428	32.911	1.00 24.83 1.00 29.92	A
ATOM	45	CD	ARG	Α	8.	39.806	-5.215	31.454	1.00 28.35	A
ATOM	46	NE	ARG	Α	8	38.409	-5.525	31.149	1.00 27.35	A A
ATOM	47	CZ	ARG	A	.8	37.467	-4.606	30.944	1.00 24.04	A
ATOM	48	NHI	ARG	A	8	36.229	-4.980	30.672	1.00 21.41	A
ATOM	49	NH2	ARG	A	8	37.768	-3.316	30.997	1.00 12.41	A
ATOM	50	С	ARG		8	41.268	-4.374	35.271	1.00 30.62	A
MOTA	51	О	ARG		8	42.402	-4.060	34.906	1.00 31.02	A
ATOM	52	N	VAL		9	41.043	-5.346	36.138	1.00 28.47	A
ATOM	53	CA	VAL		9	42.127	-6.076	36.731	1.00 25.69	A
ATOM	54	CB	VAL		9 `	42.464	-5.512	38.106	1.00 20.88	A
ATOM	55	CG1			9	43.402	-6.428	38.823	1.00 29.03	A
ATOM	56	CG2			9	43.088	-4.156	37.951	1.00 20.94	A
ATOM	57 50	C	VAL		9	41.727	-7.524	36.880	1.00 29.36	A·
ATOM	58	0	VAL		9	40.607	-7.838	37.295	1.00 27.18	A
ATOM	59	N	ILE		10	42.653	-8.401	36.507	1.00 31.47	A
ATOM ATOM	60	CA	ILE		10	42.437	-9.823	36.630	1.00 31.73	A
ATOM	61	CB	ILE		10	42.844		35.374	1.00 24.79	A
ATOM	62		ILE		10	42.634		35.554	1.00 22.18	A
ATOM	63 64	CG1			10	41.985	-10.060	34.217	1.00 28.91	A
ATOM	64 65		ILE		10	40.498	-10.358	34.363	1.00 22.28	A
ATOM	65 66	C	ILE		10	43.297		37.775	1.00 35.17	Α
ATOM	66 67		ILE		10	44.513 -		37.735	1.00 34.50	A
	67	N	TYR	A	11	42.658 -	-10.821	38.812	1.00 38.03	Α

MOTA	68	CA	TYR	A	11	43.396 -11.319 39.961 1.00 3	7.70 A
ATOM	69	CB	TYR		11	42.707 -10.949 41.266 1.00 3	
ATOM	70	CG	TYR		11	43.651 -10.957 42.435 1.00 39	9.89 A
ATOM	71		TYR		11	44.292 -9.788 42.840 1.00 44	
ATOM	72		TYR		11	45.213 -9.785 43.883 1.00 42	
ATOM	73	CD2			11	43.950 -12.135 43.107 1.00 3	
MOTA	74	CE2			11	44.876 -12.144 44.156 1.00 41	
MOTA	75	CZ	TYR		11	45.504 -10.961 44.535 1.00 41	
ATOM ATOM	76 77	OH	TYR		11	46.441 -10.942 45.544 1.00 37	
ATOM	78	C	TYR		11	43.452 -12.830 39.857 1.00 37	
ATOM	79	N O	TYR PRO		11 12	42.436 -13.498 40.048 1.00 30	
ATOM	80	CD	PRO		12	44.641 -13.385 39.534 1.00 39 45.850 -12.640 39.145 1.00 41	
ATOM	81	CA	PRO		12		
ATOM	82	CB	PRO		12		
ATOM	83	CG	PRO		12	46.270 -14.911 38.784 1.00 36 46.460 -13.558 38.135 1.00 40	
ATOM	84	C	PRO		12	44.834 -15.476 40.763 1.00 36	
ATOM	85	0	PRO		12	45.631 -15.121 41.627 1.00 35	
ATOM	86	N	ALA		13	43.909 -16.406 40.974 1.00 39	
ATOM	87	CA	ALA		13	43.824 -17.067 42.268 1.00 45	
MOTA	88	CB	ALA	A	13	42.778 -18.162 42.232 1.00 45	
MOTA	89	C	ALA	Α	13	45.196 -17.648 42.611 1.00 50	
ATOM	90	0	ALA	A	13	45 500 40 000	.35 A
ATOM	91	N	GLY	A	14	45.696 -17.306 43.795 1.00 53	
ATOM	92	CA	GLY	A	14	46.991 -17.801 44.211 1.00 53	
ATOM	93	C	GLY		14	48.012 -16.690 44.314 1.00 56	
MOTA	94	0	GLY		14	48.766 -16.635 45.286 1.00 56	_
ATOM	95	N	GLN		15	48.048 -15.809 43.313 1.00 57	
ATOM	96	CA	GLN		15	48.994 -14.697 43.307 1.00 58	
ATOM	97	CB	GLN		15	48.621 -13.682 42.228 1.00 62	.60 A
ATOM	98	CG	GLN		15	48.488 -14.259 40.834 1.00 70	.57 A
ATOM	99	CD	GLN		15	49.757 -14.154 40.013 1.00 74	
ATOM	100		GLN		15	50.828 -14.585 40.441 1.00 78	
ATOM ATOM	101 102	NE2	GLN		15	49.639 -13.585 38.815 1.00 77	_
ATOM .	103	0	GLN GLN		15	48.969 -14.010 44.665 1.00 60	
ATOM	104	N	LYS		15 16	47.905 -13.786 45.242 1.00 61	
ATOM	105	CA	LYS		16	50.140 -13.679 45.182 1.00 62 50.202 -13.015 46.469 1.00 65	
ATOM	106	CB	LYS		16		
ATOM	107	CG	LYS		16		
ATOM	108	CD	LYS		16	51.774 -12.473 48.410 1.00 80 53.238 -12.265 48.796 1.00 86	
ATOM	109	CE	LYS		16	54.125 -13.434 48.345 1.00 88	
MOTA	110	NZ	LYS		16	53.660 -14.763 48.844 1.00 90	
ATOM	111	C	LYS	Α	16	49.676 -11.597 46.316 1.00 64	
ATOM	112	0	LYS	A	16	49.138 -11.022 47.259 1.00 67	
MOTA	113	N	GLN	A	17	49.821 -11.040 45.118 1.00 61	
MOTA	114	CA	GLN		17	49.371 -9.677 44.864 1.00 58	
MOTA	115	CB	GLN	Α	17	50.213 -8.708 45.684 1.00 57	
MOTA	116	CG	GLN		17	51.678 -8.860 45.396 1.00 62	
ATOM	117	CD	GLN		17	52.461 -7.602 45.661 1.00 68	
ATOM	118		GLN		17.	52.472 -7.086 46.789 1.00 67	
MOTA	119		GLN		17	53.135 -7.092 44.618 1.00 63	
ATOM	120		GLN		17	49.452 -9.260 43.394 1.00 54	
MOTA	121	0	GLN		17	50.321 -9.709 42.656 1.00 54	.89 A
ATOM	122	N	VAL		18	48.534 -8.398 42.975 1.00 49	.56 A
ATOM	123		VAL		18	48.536 -7.900 41.613 1.00 46	.26 A
ATOM	124		VAL		18	47.223 -8.194 40.906 1.00 45	
ATOM	125	CGT	VAL	A	18	47.237 -7.586 39.519 1.00 44.	.64 A

ATOM	126		VAL		18	47.016	-9.685	40.815	1.00 46.03	A
ATOM	127	C	VAL		18	48.722	-6.397	41.729	1.00 48.04	Α -
MOTA	128	0	VAL	Α	18	48.337	-5.794	42.729	1.00 50.94	Ā
ATOM	129	N	GLN	A	19	49.321	-5.782	40.723	1.00 45.47	. A
ATOM	130	CA	GLN	Α	19	49.544	-4.359	40.794	1.00 43.17	A
ATOM	131	CB	GLN	A	19	51.035	-4.081	40.886	1.00 46.44	A
MOTA	132	CG	GLN	Α	19	51.860	-4.849	39.900	1.00 54.70	A
MOTA	133	CD	GLN	Α	19	53.307	-4.938	40.329	1.00 57.93	A
MOTA	134	OE1	GLN	A	19	53.621	-5.548	41.354	1.00 63.32	A
MOTA	1,35	NE2	GLN	A	19	54.196	-4.324	39.556	1.00 60.14	A
MOTA	136	С	GLN	Α	19	48.912	-3.578	39.660	1.00 39.45	A
MOTA	137	0	GLN	A	19	48.775	-4.074	38.554	1.00 38.04	A
MOTA	138	N	LEU	A	20	48.511	-2.350	39.981	1.00 34.78	A
MOTA	139	CA	LEU	A	20	47.857	-1.438	39.065	1.00 31.20	A
MOTA	140	CB	LEU	A	20	46.401	-1.244	39.508	1.00 26.86	A
MOTA	141	CG	LEU	A	20	45.467	-0.342	38.685	1.00 33.45	A
ATOM	142	CD1	LEU	Α	20	45.196	-0.967	37.329	1.00 24.45	A
MOTA	143	CD2	LEU	A	20	44.151	-0.144	39.432	1.00 30.84	. A
ATOM	144	C	LEU	Α	20	48.610	-0.101	39.085	1.00 32.48	A
ATOM	145	O .	LEU	Α	20	49.136	0.313	40.117	1.00 32.34	A
ATOM	146	N	ALA	A	21	48.658	0.576	37.943	1.00 33.28	A
ATOM	147	CA	ALA	Α	21	49.370	1.842	37.855	1.00 30.08	A
MOTA	148	CB	ALA	A ·	21	50.118	1.937	36.539	1.00 24.35	A
MOTA	149	С	ALA		21	48.432	3.009	37.972	1.00 31.45	A
ATOM	150	0	ALA		21	47.280	2.947	37.535	1.00 30.03	A
MOTA	151	N	VAL	Α	22	48.945	4.075	38.571	1.00 32.81	Ā
MOTA	152	CA	VAL	A	22	48.194	5.299	38.747	1.00 34.61	A
ATOM	153	CB	VAL	A	22	47.844	5.608	40.196	1.00 32.97	A
MOTA	154	CG1	VAL	Α	22	46.541	6.403	40.242	1.00 33.01	A
MOTA	155	CG2	VAL	Α	22	47.783	4.353	40.997	1.00 34.95	A
MOTA	156	C	VAL	A	22	49.150	6.378	38.341	1.00 40.85	A
ATOM	157	0	VAL		22	50.331	6.357	38.709	1.00 43.10	A
MOTA	158	N	THR	Α	23	48.631	7.341	37.605	1.00 42.34	A
ATOM	159	CA	THR	A	23	49.441	8.430	37.149	1.00 40.73	A
ATOM	160	CB	THR	Α	23	49.854	8.189	35.698	1.00 42.89	A
ATOM	161	OG1	THR	Α	23	50.298	9.418	35.118	1.00 54.11	A
ATOM	162	CG2	THR	Α	23	48.689	7.646	34.901	1.00 47.21	A
MOTA	163	C	THR	Α	23	48.635	9.708	37.290	1.00 38.53	A
ATOM	164	0	THR	A	23	47.448	9.733	36.992	1.00 35.79	A
MOTA	165	N	ASN	Α	24	49.302	10.751	37.775	1.00 40.34	A
MOTA	166	CA	ASN	A	24	48.719	12.066	37.991	1.00 40.97	A
ATOM	167	CB	ASN	\mathbf{A}	24	49.055	12.538	39.409	1.00 35.01	A
MOTA	168	CG	ASN	Α	24	48.653	13.987	39.661	1.00 43.23	A
MOTA	169	OD1	ASN	Α	24	47.764	14.517	38.999	1.00 38.96	A
MOTA	170	ND2	ASN	Α	24	49.299	14.628	40.636	1.00 41.00	A
MOTA	171	C	ASN	Α	24	49.273	13.047	36.958	1.00 47.73	A
ATOM	172	0	ASN	A	24	50.463	13.391	36.982	1.00 47.30	A
ATOM	173	N	ASN	A	25	48.396	13.483	36.056	1.00 52.99	A
MOTA	174	CA	ASN	Α	25	48.726	14.421	34.976	1.00 56.93	A
ATOM	175	CB	ASN	Α	25	47.571	14.509	33.977	1.00 55.68	A
MOTA	176	CG	ASN	A	25	47.319	13.215	33.263	1.00 53.81	A
MOTA	177	OD1	ASN	A	25	47.560	12.134	33.804	1.00 52.54	A
MOTA	178	ND2	ASN	Α	25	46.810	13.310	32.040	1.00 56:02	A
MOTA	179		ASN		25	49.007	15.836	35.454	1.00 60.12	A
MOTA	180		ASN		25	50.047	16.412	35.146	1.00 63.46	A
ATOM	181		ASP		26	48.049	16.399	36.180	1.00 60.03	A
MOTA	182		ASP		26	48.153	17.755	36.683	1.00 61.14	A
MOTA	183	CB	ASP	Α	26	47.128	17.971		1.00 63.54	A

ATOM	184	CG	ASP	Α	26	45.722	17.815	37.267	1.00 64.77	A
ATOM	185	OD1	ASP	A	26	44.792	17.913	38.093	1.00 67.45	A
MOTA	186	OD2	ASP	A	26	45.550	17.591	36.043	1.00 65.91	A
ATOM	187	C	ASP	A	26	49.521	18.147	37.180	1.00 62.42	A
MOTA	188	0	ASP	Α	26	49.892	17.878	38.317	1.00 61.06	A
MOTA	189	N	GLU	Α	27	50.256	18.809	36.302	1.00 67.35	Ā
MOTA	190	CA	GLU	A	27	51.600	19.265	36.592	1.00 71.48	A
MOTA	191	CB	GLU	Α	27	52.070	20.198	35.468	1.00 78.88	A
ATOM	192	CG	GLU	Α	27	52.499	19.441	34.200	1.00 92.01	A
MOTA	193	CD	GLU	A	27	52.239	20.197	32.899	1.00 97.34	A
ATOM	194	OE1	GLU	Α	27	52.662	21.371	32.783	1.00102.85	A
ATOM	195	OE2	GLU	A	27	51.619	19.602	31.985	1.00 99.30	A
MOTA	196	C	GLU	A	27	51.719	19.952	37.942	1.00 69.71	A
MOTA	197	0	GLU	Α	27	52.804	20.009	38.506	1.00 69.50	A
ATOM	198	N	ASN	A	28	50.616	20.461	38.477	1.00 68.96	A
ATOM	199	CA	ASN	Α	28	50.704	21.135	39.759	1.00 71.52	A
ATOM	200	CB	ASN	Α	28	51.186	22.579	39.555	1.00 77.25	A
MOTA	201	CG	ASN	A	28	50.385	23.327	38.497		A
ATOM	202	OD1	ASN	A	28	50.786	24.402	38.043	1.00 80.59	A
ATOM	203	ND2	ASN	Α	28	49.245	22.760	38.101	1.00 82.72	A
ATOM	204	C	ASN	Α	28	49.422	21.112	40.562	1.00 70.70	A
ATOM	205	0	ASN	Α	28	48.511	21.901	40.340	1.00 74.18	A
ATOM	206	N	SER	Α	29	49.383	20.196	41.515	1.00 70.28	A
ATOM	207	CA	SER	Α	29	48.245	19.999	42.405	1.00 69.73	A
ATOM	208	CB	SER	A	29	46.925	20.032	41.623	1.00 70.95	A
MOTA	209	QG	SER	A	29	46.897	19.035	40.618	1.00 69.06	A
MOTA	210	С	SER	Α	29	48.442	18.621	43.034	1.00 66.59	A
MOTA	211	0	SER	A	29	48.460	17.610	42.338	1.00 66.98	A
ATOM	212	N	THR	Α	30	48.613	18.581	44.346	1.00 62.94	A
MOTA	213	CA	THR	Α	30	48.822	17.312	45.010	1.00 58.80	A
MOTA	214	CB	THR	Α	30	49.488	17.515	46.376	1.00 60.11	A
ATOM	215	OG1	THR	A	30	50.669	18.313	46.221	1.00 60.81	. A
MOTA	216	CG2	THR	A	30	49.903	16.189	46.957	1.00 65.77	A
ATOM .	21,7	C	THR	A	30	47.497	16.590	45.189	1.00 55.15	A
MOTA	218	0	THR	Α	30	46.431	17.197	45.103	1.00 57.03	A
MOTA	219	N	TYR	Α	31	47.567	15.285	45.410	1.00 51.62	A
MOTA	220	CA	TYR		31	46.373	14.470	45.618	1.00 48.42	A
MOTA	221	CB	TYR	A	31	45.941	13.790	44.327	1.00 47.52	A
ATOM	222	CG	TYR		31	45.261	14.681	43.331	1.00 51.38	. A
ATOM	223	CD1	TYR	Α	31	45.867	14.994	42.113	1.00 50.92	A
MOTA	224	CE1	TYR	A	31	45.201	15.749	41.162	1.00 54.59	A
MOTA	225	CD2	TYR	A	31	43.975	15.153	43.570	1.00 53.90	A
MOTA	226	CE2	TYR		31	43.300	15.905	42.623	1.00 54.60	A
MOTA	227	CZ	TYR		31	43.916	16.196	41.425	1.00 56.01	A
ATOM	228	OH	TYR		31	43.234	16.912	40.479	1.00 63.46	A
MOTA	229	С	TYR		31 .	46.614	13.378	46.647	1.00 46.00	A
ATOM	230	0	TYR		31	47.735	12.910	46.845	1.00 48.20	A
MOTA	231	N	LEU		32	45.550	12.981	47.317	1.00 43.61	A
ATOM	232	CA	LEU		32	45.641	11.913	48.283	1.00 42.05	A
ATOM	233	CB	LEU		32	44.907	12.268	49.569	1.00 48.78	A
ATOM	234	CG	LEU		32	45.708	13.010	50.632	1.00 52.70	A
MOTA	235		LEU		32	44.766	13.447	51.753	1.00 53.82	A
ATOM	236		LEU		32	46.827	12.107	51.153	1.00 46.91	A
ATOM	237	C	LEU		32	44.934	10.770	47.599	1.00 43.83	A
ATOM	238	0	LEU		32	43.762	10.878	47.214	1.00 40.62	A
ATOM	239	N	ILE		33	45.660	9.682	47.417	1.00 42.76	A
ATOM	240	CA	ILE		33	45.088	8.525	46.775	1.00 38.12	A
ATOM	241	CB	ILE	A	33	46.139	7.822	45.911	1.00 36.49	A

ATOM	242	CG2			33	45.513	6.655	45.157	1.00 40.10	A
MOTA	243	CGI	ILE	A	33	46.762	8.846	44.959	1.00 38.79	A
ATOM	244	CD1	ILE	Α	33	45.752	9.675	44.183	1.00 28.86	A
MOTA	245	· C	ILE	Α	33	44.591	7.598	47.859	1.00 35.40	A
ATOM	246	0	ILE	A	33	45.333	7.224	48.760	1.00 36.59	A
MOTA	247	N	GLN		34	43.321	7.249	47.770	1.00 33.93	A
MOTA	248	CA	GLN		34	42.688	6.358	48.730	1.00 35.55	A
ATOM	249	CB	GLN		34	41.659	7.135	49.539	1.00 40.32	A
MOTA	250	CG	GLN	A	34	41.417	6.623	50.923	1.00 41.00	A
MOTA	251	CD	GLN	A	34	40.494	7.533	51.692	1.00 45.44	A
ATOM	252		GLN		34	39.329	7.700	51.335	1.00 52.79	A
ATOM	253	NE2			34	41.013	8.145	52.746	1.00 47.22	A
ATOM	254	C	GLN		34	41.997	5.291	47.895	1.00 33.40	A
MOTA	255	0	GLN		34	41.079	5.594	47.143	1.00 32.21	A
MOTA	256	N	SER		35	42.431	4.045	48.036	1.00 32.83	A
ATOM	257	CA	SER		35	41.864	2.961	47.249	1.00 32.88	A
MOTA	258	CB	SER		35	42.968	2.340	46.398	1.00 38.87	A
ATOM	259	OG	SER		35	43.755	3.350	45.799	1.00 47.39	A
ATOM	260	C	SER		35	41.214	1.869	48.077	1.00 30.90	A
ATOM	261	0	SER		35	41.593	1.643	49.215	1.00 39.12	A
ATOM	262	N	TRP		36	40.240	1.182	47.502	1.00 25.03	A
ATOM	263	CA	TRP		36	39.580	0.082	48.198	1.00 25.04	A
ATOM	264	CB	TRP		36	38.594	0.587	49.257	1.00 18.25	A
ATOM	265	CG	TRP		36	37.338	1.180	48.706	1.00 20.02	A
ATOM	266		TRP		36	37.158	2.524	48.248	1.00 16.95	A
ATOM	267		TRP		36	35.827	2.630	47.772	1.00 22.43	A
ATOM	268	CE3			36	37.989	3.650	48.198	1.00 11.35	A
ATOM	269	CD1			36	36.151	0.540	48.497	1.00 21.69	A
ATOM	270	NE1	TRP		36	35.235	1.404	47.936	1.00 24.21	A
ATOM	271	CZ2	TRP		36	35.303	3.829	47.247	1.00 17.19	A
ATOM	272	CZ3	TRP		36	37.465	4.857	47.678	1.00 15.18	A
ATOM	273	CH2	TRP		36	36.132	4.931	47.212	1.00 10.97	A
ATOM ATOM	274 275	C	TRP		36	38.853	-0.797	47.189	1.00 25.22	A
ATOM	275	O N	TRP		36 37	38.759	-0.476	46.007	1.00 24.89	A
ATOM	277	N CA	VAL VAL		37 37	38.343	-1.915	47.666	1.00 24.80	A
ATOM	278	CB	VAL		37	37.654	-2.836	46.805	1.00 26.60	Α
ATOM	279		VAL		37 37	38.524 37.783	-4.070	46.531	1.00 28.07	A
ATOM	280		VAL		37	39.828	-5.034	45.631	1.00 29.46	A
ATOM	281	C	VAL		37	36.358	-3.640 -3.279	45.893 47.452	1.00 26.19	A
ATOM	282	õ	VAL		37	36.353	-3.783	47.452	1.00 26.97 1.00 32.49	A
ATOM	283	N	GLU		38	35.263	-3.086	46.737	1.00 32.49	A
ATOM	284	CA	GLU		38	33.958	-3.484	47.218	1.00 25.19	A A
ATOM	285	CB	GLU		38	32.929	-2.426	46.850	1.00 23.19	
ATOM	286	CG	GLU		38	33.247	-1.083	47.474	1.00 29.25	A A
ATOM	287	CD	GLU		38	32.394	0.013	46.925	1.00 23.23	A
ATOM	288	OE1			38	31.336	-0.340	46.357	1.00 33.29	Ā
ATOM	289	OE2	GLU		38.	32.769	1.208	47.067	1.00 29.73	Ā
ATOM	290	C	GLU		38	33.650	-4.782	46.515	1.00 27.91	Ā
ATOM	291	0	GLU		38	34.249	-5.077	45.482	1.00 30.92	A
MOTA	292	N	ASN		39	32.751	-5.578	47.082	1.00 27.23	A
ATOM	293	CA	ASN		39	32.397	6.825	46.438	1.00 28.78	A
ATOM	294	CB	ASN		39	31.982	-7.889	47.451	1.00 31.06	Ā
ATOM	295	CG	ASN		39	30.711	-7.533	48.199	1.00 41.12	A
MOTA	296	OD1			39	29.906	-6.709	47.749	1.00 41.67	Ā
MOTA	297	ND2			39	30.513	-8.176	49.344	1.00 42.07	A
ATOM	298	C	ASN		39	31.262	-6.551	45.467	1.00 30.36	A
MOTA	299	0	ASN	Α	39	30.858	-5.403	45.288	1.00 28.38	A

MOTA	300	N	ALA	A	40	30.748	-7.613	44.852	1.00 33.88	А
MOTA	301	CA	ALA	Α	40	29.691	-7.489	43.867	1.00 32.53	A
MOTA	302	CB	ALA	Α	40	29.265	-8.847	43.402	1.00 36.04	A
MOTA	303	C	ALA	Α.	40	28.502	-6.716	44.375	1.00 34.18	A
ATOM	304	0	ALA	A	40	27.903	-5.952	43.634	1.00 37.55	A
ATOM	305	N	ASP	A	41	28.154	-6.897	45.638	1.00 35.10	A
ATOM	306	CA	ASP	Α	41	27.018	-6.172	46.172	1.00 40.17	A
MOTA	307	CB	ASP	Α	41	26.436	-6.907	47.367	1.00 46.82	A
MOTA	308	CG	ASP	Α	41	25.760	-8.197	46.967	1.00 51.21	A
MOTA	309	OD1	ASP	Α	41	24.921	-8.152	46.045	1.00 54.74	A
ATOM	310	OD2	ASP	Α	41	26.062	-9.247	47.569	1.00 49.46	A
MOTA	311	C	ASP	A	41	27.314	-4.731	46.548	1.00 41.50	A
ATOM	312	0	ASP		41	26.434	-4.026	47.017	1.00 47.75	A
MOTA	313	N	GLY	Α	42	28.546	-4.287	46.340	1.00 38.41	A
MOTA	314	CA	GLY	A	42	28.880	-2.915	46.654	1.00 31.80	A
MOTA	315	C	GLY		42	29.339	-2.711	48.073	1.00 31.58	A
ATOM	316	0	GLY		42	29.633	-1.591	48.461	1.00 32.94	A
MOTA	317	N	VAL		43	29.415	-3.772	48.864	1.00 33.94	A
ATOM	318	CA	VAL		43	29.857	-3.585	50.235	1.00 35.74	A
ATOM	319	CB	VAL		43	29.086	-4.505	51.225	1.00 30.70	A
ATOM	320		VAL		43	27.956	-5.203	50.524	1.00 32.32	A
ATOM	321		VAL		43	30.021	-5.481	51.878	1.00 32.27	A
ATOM	322	C	VAL		43	31.366	-3.770	50.406	1.00 40.26	A
ATOM	323	ō	VAL		43	31.984	-4.648	49.782	1.00 40.24	
MOTA	324	N	LYS		44	31.950	-2.922	51.252	1.00 40.24	A
ATOM	325	CA	LYS		44	33.372	-2.977	51.510	1.00 38.14	A
MOTA	326	CB	LYS		44	33.873	-1.658	52.115		A
ATOM	327	CG	LYS		44	33.689	-0.406		1.00 38.71	A
ATOM	328	CD	LYS		44	32.808	0.593	51.277 51.997	1.00 38.64	A
ATOM	329	CE	LYS		44	32.660	1.863	51.211	1.00 45.19	A
MOTA	330	NZ	LYS		44	33.992			1.00 44.21	A
ATOM	331	C	LYS		44	33.729	2.459	51.006	1.00 53.47	A
ATOM	332	Õ	LYS		44	33.729	-4.101	52.472	1.00 40.34	A
ATOM	333	N	ASP		45		-3.864	53.668	1.00 41.16	A
MOTA	334	CA	ASP		45	33.796 34.236	-5.334	51.988	1.00 41.72	A
ATOM	335	CB	ASP		45		-6.399	52.879	1.00 42.88	. A
ATOM	336	CG	ASP		45	33.736	-7.766	52.441	1.00 45.54	A
ATOM	337		ASP		45	33.828	-7.973	50.952	1.00 45.53	A
ATOM	338		ASP		45	34.746	-7.404	50.328	1.00 46.24	A
ATOM	339	C	ASP		45	32.983 35.739	-8.722	50.416	1.00 39.44	A
ATOM	340	o	ASP		45	36.246	-6.311 -5.430	52.728	1.00 46.78	A
ATOM	341	N	GLY		46			52.019	1.00 52.22	A
MOTA	342	CA	GLY		46	36.477	-7.204	53.355	1.00 46.85	A
ATOM	343	C	GLY		46	37.917	-7.067 -8.097	53.229	1.00 44.85	A
ATOM	344	Ö	GLY		46	38.525		52.322	1.00 43.84	A
ATOM	345	И	ARG		47	39.712	-8.393	52.444 51.412	1.00 42.91	A
ATOM	346	CA	ARG		47	37.718	-8.641 -9.659		1.00 41.43	A
ATOM	347	CB	ARG		47	38.204		50.507	1.00 39.36	A
ATOM	348	CG	ARG		47			49.473 49.699	1.00 48.60	A
ATOM	349	CD	ARG				-11.347		1.00 59.40	A
ATOM					47		-11.368	50.952	1.00 67.93	A
ATOM	350	NE	ARG		47		-12.718	51.234	1.00 81.01	A
ATOM	351	CZ	ARG		47		-13.664	51.793	1.00 88.24	A
	352		ARG		47		-13.398	52.135	1.00 92.78	A
ATOM	353		ARG		47		-14.880	52.005	1.00 91.41	A
ATOM	354	C	ARG		47	39.498	-9.260	49.828	1.00 38.41	A
ATOM	355	0	ARG		47		-10.092	49.608	1.00 36.37	A
ATOM	356	N	PHE		48	39.633	-7.983	49.504	1.00 35.37	A
MOTA	357	CA	PHE	A	48	40.851	-7.518	48.862	1.00 35.98	Α

MOTA	358	CB	PHE		48	40.635	-7.303	47.352	1.00 33.65	A
ATOM	359	CG	PHE		48	40.439	-8.571	46.602	1.00 31.31	A
ATOM	360		PHE		48	39.172	-9.129	46.481	1.00 33.95	A
ATOM	361		PHE		48	41.537	-9.272	46.109	1.00 32.43	A
ATOM	362		PHE		48	39.000	-10.378	45.891	1.00 32.81	A
ATOM	363	CE2	PHE		48	41.383	-10.514	45.520	1.00 31.82	Α
ATOM	364	CZ	PHE		48	40.116	-11.077	45.409	1.00 30.28	A
ATOM	365	C	PHE		48	41.320	-6.237	49.512	1.00 34.18	A
MOTA	366	0	PHE		48	40.505	-5.423	49.906	1.00 31.01	A
ATOM	367	N	ILE		49	42.635	-6.061	49.609	1.00 35.45	A
ATOM	368	CA	ILE		49	43.191	-4.871	50.225	1.00 36.92	A
ATOM	369	CB	ILE		49	43.813	-5.224	51.582	1.00 42.20	A
ATOM	370	CG2	ILE		49	44.465	-4.001	52.221	1.00 35.45	A
ATOM	371	CG1	ILE		49	42.701	-5.733	52.499	1.00 44.49	A
ATOM	372	CD1	ILE		49	43.201	-6.508	53.688	1.00 53.29	A
ATOM	373	C	ILE		49	44.209	-4.245	49.304	1.00 35.56	Α
ATOM	374	0	ILE		49	45.009	-4.933	48.685	1.00 39.65	A
ATOM	375	N	VAL		50	44.175	-2.927	49.215	1.00 32.29	A
ATOM	376	CA	VAL		50	45.071	-2.211	48.330	1.00 33.81	A
ATOM	377	CB	VAL		50	44.279	-1.218	47.435	1.00 35.53	A
MOTA	378	CG1			50	45.207	-0.573	46.421	1.00 37.38	A
MOTA	379		VAL		50	43.125	-1.937	46.741	1.00 37.16	Α
ATOM	380	C	VAL		50	46.067	-1.423	49.143	1.00 35.47	A
MOTA	381	0	VAL		50	45.720	-0.887	50.188	1.00 39.81	A
MOTA	382	N	THR		51	47.304	-1.351	48.671	1.00 35.54	. A
MOTA	383	CA	THR		51	48.327	-0.580	49.365	1.00 34.50	\mathbf{A}
ATOM	384	CB	THR		51	49.338	-1.464	50.123	1.00 37.75	A
ATOM ATOM	385 386	OG1 CG2	THR		51	49.924	-2.404	49.213	1.00 44.60	. A
ATOM	387	CGZ	THR		51 51	48.677	-2.205	51.261	1.00 46.16	A
ATOM	388	0	THR		51	49.122	0.214	48.350	1.00 34.70	A
ATOM	389	N	PRO		51 52	49.304	-0.209	47.211	1.00 35.22	A
ATOM	390	CD	PRO		52 52	49.561	1.406	48.738	1.00 34.51	A
MOTA	391	CA	PRO		52	50.735 49.274	2.071	48.158	1.00 30.64	A
ATOM	392	CB	PRO		52	50.259	1.930	50.075	1.00 34.32	A
ATOM	393	CG	PRO		52	50.667	3.090	50.220	1.00 32.25	A
ATOM	394	C	PRO		52	47.832	3.407 2.392	48.819	1.00 36.50	A
ATOM	395	ō	PRO		52	47.312	2.392	50.157 49.223	1.00 34.16	A
ATOM	396	N	PRO		53	47.161	2.115	51.275	1.00 39.05	A
	397	CD	PRO		53	47.651	1.487	52.513	1.00 32.08	A
ATOM	398	CA	PRO		53	45.765	2.538	51.410	1.00 27.65 1.00 30.20	A
ATOM	399	CB	PRO		53	45.386	2.020	52.790	1.00 30.20	A A
ATOM	400	CG	PRO		53	46.713	2.043	53.534	1.00 31.39	A
ATOM	401	C	PRO		53	45.552	4.047	51.286	1.00 30.89	A
MOTA	402	Ō	PRO		53	44.445	4.490	51.000	1.00 30.55	A
ATOM	403	N	LEU		54	46.610	4.830	51.499	1.00 30.33	A
ATOM	404	CA	LEU		54	46.525	6.290	51.434	1.00 32.42	A
ATOM	405	CB	LEU	Α	54	45.980	6.838	52.737	1.00 35.06	A
MOTA	406	CG	LEU	Α	54	45.866	8.355	52.833	1.00 35.56	' A
ATOM	407	CD1	LEU	Α	54	44.602	8.812	52.104	1.00 39.67	A
MOTA	408	CD2	LEU	Α	54	45.807	8.757	54.291	1.00 34.78	A
ATOM	409	C	LEU		54	47.883	6.920	51.222	1.00 35.61	A
ATÓM	410	0	LEU	A	54	48.789	6.720	52.035	1.00 40.67	A
MOTA	411	N	PHE	A	55	48.028	7.705	50.162	1.00 33.82	A
MOTA	412	CA	PHE		55	49.313	8.339	49.878	1.00 36.60	A
MOTA	413	CB	PHE	A	55	50.263	7.343	49.227	1.00 35.58	A
MOTA	414	CG	PHE		55	49.797	6.856	47.895	1.00 40.56	A
ATOM	415	CD1	PHE	A	5 5	50.227	7.467	46.720	1.00 42.70	A

MOTA	416		PHE		55	48.903	5.799	47.813	1.00 44.00	A
MOTA	417	CE1			55	49.768	7.029	45.471	1.00 46.06	A
ATOM	418	CE2	PHE	Α	55	48.435	5.352	46.575	1.00 50.94	A
ATOM	419	CZ	PHE		55	48.869	5.969	45.397	1.00 48.90	A
MOTA	420	C	PHE	A	55	49.160	9.534	48.968	1.00 40.04	A
ATOM	421	0	PHE	Α	55	48.120	9.706	48.316	1.00 43.34	A
MOTA	422	N	ALA	Α	56	50.210	10.351	48.904	1.00 40.28	A
MOTA	423	CA	ALA	A	56	50.169	11.551	48.078	1.00 39.73	A
MOTA	424	CB	ALA	Α	56	50.683	12.732	48.873	1.00 34.93	A
MOTA	425	C	ALA	Α	56	50.910	11.456	46.746	1.00 39.80	A
ATOM	426	0	ALA		56	51.923	10.768	46.613	1.00 39.90	A
MOTA	427	N	MET		57	50.370	12.146	45.753	1.00 39.84	A
MOTA	428	CA	MET	Α	57	50.974	12.205	44.437	1.00 40.80	A
MOTA	429	CB	MET	Α	57	50.090	11.534	43.389	1.00 39.08	A
MOTA	430	CG	MET		57	49.830	10.075	43.654	1.00 39.96	A
MOTA	431	SD	MET		57	49.830	9.123	42.135	1.00 45.17	A
MOTA	432	CE	MET		57	48.384	9.770	41.389	1.00 52.26	A
ATOM	433	C	MET		57	51.083	13.695	44.163	1.00 43.85	A
MOTA	434	0	MET		57	50.077	14.380	43.948	1.00 41.80	A
MOTA	435	N	LYS		58	52.310	14.196	44,.200	1.00 47.84	A
MOTA	436	CA	LYS		58	52.555	15.608	43.974	1.00 54.71	A
ATOM	437	CB	LYS		58	53.646	16.094	44.920	1.00 60.11	A
ATOM	438	CG	LYS		58	53.694	17.598	45.085	1.00 67.21	A
ATOM	439	CD	LYS		58	54.848	18.011	45.988	1.00 71.96	·A
ATOM	440	CE	LYS		58	54.593	19.369	46.633	1.00 76.40	A
ATOM	441	NZ	LYS		58	53.433	19.316	47.578	1.00 75.23	A
ATOM	442	C	LYS		58	52.965	15.879	42.535	1.00 57.17	A
ATOM	443	0	LYS		58	53.984	15.372	42.068	1.00 60.73	A
ATOM	444	N	GLY		59	52.169	16.683	41.835	1.00 57.99	A
ATOM	445	CA	GLY		59	52.479	17.009	40.454	1.00 56.05	A
ATOM	446	C	GLY		59	52.534		39.588	1.00 51.99	A
MOTA	447	0	GLY		59	52.151	14.698	40.037	1.00 47.22	A
MOTA	448	N	LYS		60	53.011	15.914	38.353	1.00 53.30	A
ATOM. ATOM	449 450	CA CB	LYS		60	53.090	14.782	37.435	1.00 56.47	A
ATOM	451	CG	LYS		60 60	53.648	15.213	36.073	1.00 54.61	A
ATOM	452	CD	LYS		60	52.831	16.302	35.394	1.00 55.52	, A
ATOM	453	CE	LYS		60	52.966	16.264	33.883	1.00 60.88	` A .
ATOM	454	NZ	LYS		60	52.305 52.298	15.019	33.306	1.00 69.72	A
ATOM	455	C	LYS		60	53.973	14.996 13.715	31.812 38.049	1.00 76.32	A
ATOM	456	ō	LYS		60	55.185	13.880	38.144	1.00 56.25 1.00 58.88	A
ATOM	457	N	LYS		61	53.347	12.626	38.475	1.00 51.75	A
ATOM	458	CA	LYS		61	54.047	11.521	39.111	1.00 47.89	A
ATOM	459	СВ	LYS		61	53.939	11.629	40.636	1.00 46.44	A A
ATOM	460	CG	LYS		61	55.271	11.738	41.355	1.00 54.37	A
ATOM	461	CD	LYS		61	55.358	10.753		1.00 59.29	A
ATOM	462	CE	LYS		61	54.288	11.027	43.578	1.00 70.05	. A
ATOM	463	NZ	LYS		61	54.257	9.991	44.675	1.00 68.00	A
ATOM	464	C	LYS		61	53.409	10.217	38.655	1.00 47.76	A
ATOM	465	0	LYS		61	52.373	10.215	37.990	1.00 45.68	A
ATOM	466	N	GLU		62	54.031	9.105	39.011	1.00 47.60	A
ATOM	467	CA	GLU		62	53.503	7.801	38.642	1.00 47.62	A
MOTA	468	СВ	GLU		62	54.140	7.341	37.336	1.00 50.03	A
ATOM	469	CG	GLU		62	53.200	6.560	36.450	1.00 66.86	A
ATOM	470	CD	GLU		62	53.442	5.062	36.505	1.00 73.59	A
MOTA	471	OE1	GLU	Α	62	53.477	4.498	37.622	1.00 79.17	A
MOTA	472		GLU		62	53.593	4.449	35.424	1.00 74.00	A
MOTA	473	С	GLU		62	53.855	6.861	39.787	1.00 44.41	A

ATOM	474	0	GLU		62	54.98	1 6.872	40.276	1.00 49.60	A
MOTA	475	N	ASN	Α	63	52.89			1.00 39.52	A
MOTA	476	CA	ASN	Α	63	53.16	8 5.176		1.00 39.57	A
ATOM	477	CB	ASN	Α	63	52.70	5 5.728	42.701	1.00 45.23	A
MOTA	478	CG	ASN	A	63	53.43	2 6.976	43.104	1.00 50.88	A
ATOM	479		ASN		63	53.00		42.783	1.00 55.66	A
MOTA	480	ND2	ASN	A	63	54.543	6.811	43.807	1.00 53.75	A
ATOM	481	C	ASN	A	63	52.42	3.914	41.099	1.00 39.45	A
MOTA	482	0	ASN	A	63	51.608	3.847	40.170	1.00 40.86	A
MOTA	483	N	THR	A	64	52.668	3 2.921	41.946	1.00 36.67	A
MOTA	484	CA	THR	Α	64	52.008	3 1.643	41.789	1.00 36.69	A
MOTA	485	CB	THR		64	53.013	0.536	41.545	1.00 34.21	A
ATOM	486	OG1			64	53.87	7 0.908	40.465	1.00 46.99	A
MOTA	487	CG2			64	52.291	L -0.755	41.206	1.00 30.34	A
MOTA	488	C	THR		64	51.144		42.947	1.00 37.73	A
MOTA	489	0	THR		64	51.566		44.099	1.00 41.52	A
ATOM	490	N	LEU		65	49.927		42.620	1.00 36.85	A
ATOM	491	CA	LEU		65	49.000		43.610	1.00 37.00	A
MOTA	492	CB	LEU		65	47.577		43.250	1.00 32.71	A
ATOM	493	CG	LEU		65	47.260		43.370	1.00 28.50	A
ATOM	494		LEU		65	45.806		43.080	1.00 24.00	A
ATOM	495	CD2			65	47.589		44.765	1.00 34.11	A
MOTA MOTA	496	C	LEU		65	49.130		43.571	1.00 39.68	A
ATOM	497 498	O	LEU		65	49.247		42.495	1.00 40.31	A
MOTA	499	N CA	ARG		66	49.136		44.736	1.00 41.29	A
ATOM	500	CB	ARG ARG		66	49.247		44.807	1.00 42.44	A
MOTA	501	CG	ARG		66 66	50.493		45.598	1.00 46.83	A
ATOM	502	CD	ARG		66	51.785 52.972		44.998	1.00 55.38	A
ATOM	503	NE	ARG		66	54.080		45.918	1.00 63.92	A
ATOM	504	CZ	ARG		66	54.820		45.647	1.00 65.49	A
ATOM	505		ARG		66	54.573		44.545 43.609	1.00 64.91	A
ATOM	506		ARG		66	55.795		44.375	1.00 67.73 1.00 66.42	A
ATOM	507	C	ARG		66	48.007		45.483	1.00 43.47	A
MOTA	508	0	ARG.		66	47.672		46.597	1.00 46.99	A A
MOTA	509	N	ILE	Α	67	47.322		44.798	1.00 40.54	Ā
MOTA	510	CA	ILE	Α	67	46.104		45.325	1.00 40.90	Ä
MOTA	511	CB	ILE	Α	67	45.059		44.215	1.00 39.11	A
MOTA	512	CG2	ILE	Α	67	43.889	-6.423	44.783	1.00 41.97	A
MOTA	513	CG1	ILE	A	67	44.558	-4.336	43.626	1.00 40.04	A
MOTA	514	CD1	ILE	A	67	45.499	-3.707	42.659	1.00 40.41	A
ATOM	515	С	ILE	Α	67	46.405	-6.738	46.002	1.00 43.96	A
MOTA	516	0	ILE		67	46.889	-7.687	45.371	1.00 45.99	A
MOTA	517	И	LEU		68	46.090	-6.819	47.285	1.00 41.33	A
ATOM	518	CA	LEU		68	46.349		48.036	1.00 41.16	A
MOTA	519	CB	LEU		68	46.990		.49.367	1.00.42.94	Α
MOTA	520	CG	LEU		68	48.140		49.331	1.00 39.91	A
ATOM	521		LEU		68	48.575		50.750	1.00 42.26	A
MOTA MOTA	522		LEU		68	49.279		48.500	1.00 42.74	Α
ATOM	523 524	C	LEU		68	45.110	=	48.302	1.00 43.60	A
ATOM	525	O N	ASP		68	44.056		48.684	1.00 38.41	A
ATOM	526	N CA	ASP		69		-10.159	48.118	1.00 46.41	. A
ATOM	527	CB	ASP		69		-11.148	48.324	1.00 45.81	A
MOTA	52 <i>1</i> 528	CG	ASP		69 69		-12.421	47.594	1.00 45.36	A
ATOM	529		ASP		69		-13.568	47.814	1.00 49.76	Α.
ATOM	530		ASP		69		-14.639 -13.409	47.200	1.00 49.67	A
ATOM	531	C	ASP		69		-13.409	48.592	1.00 37.19	A
	J J 4.	-			09	44.0//	-11.413	49.816	1.00 50.70	A

MOTA	532	0	ASP		69	44.955 -		50.451	1.00 55.74	A
MOTA	533	N	ALA	Α	70	42.962 -		50.388	1.00 56.46	A
MOTA	534	CA	ALA	Α	70	42.732 -	11.239	51.803	1.00 63.86	A
ATOM	535	CB	ALA	A	70	42.069 -	10.041	52.441	1.00 64.03	. A
ATOM	536	C	ALA	A	70	41.829 -	12.452	51.918	1.00 71.40	A
ATOM	537	0	ALA		70	41.856 -	13.178	52.914	1.00 73.20	A
MOTA	538	N	THR	Α	71	41.025 -	12.664	50.879	1.00 79.04	A
ATOM	539	CA	THR	Α	71	40.097 -	13.786	50.838	1.00 85.26	A
MOTA	540	CB	THR	Ά	71	39.150 -	13.712	49.604	1.00 82.93	Α
MOTA	541	OG1			71	38.343 -	14.895	49.554	1.00 83.04	A
MOTA	542	CG2	THR	A	71	39.935 ~	13.586	48.308	1.00 81.32	A
MOTA	.543	C	THR		71	40.843 -	15.111	50.817	1.00 91.33	A
ATOM	544	0	THR		71	41.361 -		49.775	1.00 92.62	A
MOTA	545	N	ASN		72	40.901 -		51.980	1.00 95.07	A
ATOM	546	CA	ASN		72	41.577 -	17.039	52.114	1.00 99.70	A
ATOM	547	CB	asn		7.2		17.458	53.590	1.00104.68	A
ATOM	548	CG	asn		72	42.720 -		54.370	1.00108.97	Α
ATOM	549		ASN		72	42.890 -		55.573	1.00109.76	A
ATOM	550		ASN		72	43.478 -		53.687	1.00109.90	A
ATOM	551	C	ASN		72	40.888 -		51.286	1.00100.06	A
ATOM	552	0	ASN		72	40.287 -		51.836	1.00101.61	A
ATOM	553	N	ASN		73	40.976 -		49.964	1.00 98.34	A
ATOM	554	CA	ASN		73	40.365 -		49.058	1.00 95.26	A
ATOM	555	CB	ASN		73	41.224 -		48.985	1.00 97.32	A
ATOM	556	CG	ASN		73	42.714 -		48.919	1.00 98.90	A
ATOM	557		ASN		73	43.299 -		49.866	1.00 99.05	A
MOTA	558		ASN		73	43.336 ~		47.799	1.00 97.95	A
ATOM ATOM	559	C	ASN		73	38.955 -		49.535	1.00 91.54	А
ATOM	560 561	0	ASN		73	38.537 -		49.424	1.00 91.21	A
ATOM	561 562	N CA	GLN		74 74		18.366	50.074	1.00 85.54	A
ATOM	563	CB	GLN		74	36.877 -		50.570	1.00 80.08	A
ATOM	564	CG	GLN		74 74	36.630 -		51.813	1.00 86.66	A
ATOM	565	CD	GLN		74 74	37.586 -		52.980	1.00 95.33	A
ATOM	566		GLN		74	37.648 - 38.367 -		54.059	1.00 98.36	A
MOTA	567		GLN		74	36.902 -		55.055 53.858	1.00 96.31	A
ATOM	568	C	GLN		74	35.855 -		49.485	1.00 97.60	A
ATOM	569	ō.	GLN		74	34.654 -		49.751	1.00 72.34 1.00 70.12	A
ATOM	570	N	LEU		75	36.348 -		48.258	1.00 70.12	A
ATOM	571	CA	LEU		75		17.789	47.112	1.00 58.03	A A
ATOM	572	CB	LEU		75	36.149 -		46.263	1.00 48.34	A
MOTA	573	CG	LEU		75	36.387 -		46.882	1.00 41.97	A
MOTA	574	CD1	LEU		75		14.547	46.017	1.00 33.36	A
ATOM	575		LEU		75		14.567	47.043	1.00 39.69	A
MOTA	576	C	LEU		75		19.007	46.228	1.00 58.98	A
MOTA	577	0	LEU	Α	75	36.066 -		46.282	1.00 61.87	A
MOTA	578	N	PRO		76	34.247 -		45.399	1.00 57.76	A
MOTA	579	CD	PRO		76	33.179 -		45.323	1.00 59.33	A
MOTA	580	CA	PRO	A	76	33.968 -		44.497	1.00 59.21	·A
ATOM	581	CB	PRO	Α	76	32.805 -		43.663	1.00 55.89	A
ATOM	582	CG	PRO	Α	76	32.069 -		44.630	1.00 54.17	A
MOTA	583	С	PRO		76	35.216 -		43.645	1.00 62.11	A
ATOM	584	0	PRO	Α	76	35.864 -		43.192	1.00 61.27	A
MOTA	585	N	GLN	Α	77	35.545 -		43.423	1.00 64.43	A
ATOM •	586	CA	ĠľW		77 .	36.729 -	22.004	42.641	1.00 65.67	A
ATOM	587	CB	GLN		77	37.551 -		43.391	1.00 66.33	A
ATOM	588	CG	GLN	Α	77	38.102 -	22.528	44.697	1.00 70.54	A
ATOM	589	CD	GLN	Α	77	38.920 -			1.00 74.29	A

ATOM	590		GLN		77			-20.279	45.225	1.00 72.21	A
ATOM	591		GLN		77			-21.299	43.529	1.00 74.12	A
ATOM	592	C	GLN		77			-22.480	41.210	1.00 64.93	A
ATOM	593	0	GLN		77			-22.800	40.482	1.00 64.36	A
ATOM	594	N	ASP		78			-22.501	40.804	1.00 62.06	A
ATOM	595	CA	ASP		78			-22.936	39.463	1.00 59.81	A
ATOM ATOM	596	CB	ASP		78			-23.819	39.522	1.00 60.16	A
ATOM	597 598	CG	ASP ASP		78			23.128	40.186	1.00 64.25	A
ATOM	599		ASP		78 70			23.598	40.011	1.00 67.41	A
MOTA	600	C	ASP		78 78			-22.122	40.894	1.00 68.85	A
ATOM	601	Õ	ASP		78			-21.773 -21.954	38.504	1.00 60.48	A
ATOM	602	N	ARG		79			-21.334	37.284	1.00 61.48	A
ATOM	603	CA	ARG		79			-19.401	39.053	1.00 59.75	A
ATOM	604	CB	ARG		79			-19.186	38.239 38.221	1.00 53.65	A
ATOM	605	CG	ARG		79			-18.866	39.599	1.00 53.59 1.00 53.65	A
ATOM	606	CD	ARG		79			-19.089	39.651	1.00 53.65	A.
ATOM	607	NE	ARG		79			-20.515	39.592	1.00 59.91	A A
ATOM	608	CZ	ARG		79			-21.040	39.393	1.00 59.96	A A
ATOM	609	NH1	ARG	A	79			-20.255	39.230	1.00 56.86	Â
ATOM	610	NH2	ARG	Α	.79			-22.360	39.346	1.00 60.89	A
MOTA	611	C	ARG	A	79			-18.175	38.819	1.00 48.41	A
ATOM	612	0	ARG	Α	79			-18.212	39.935	1.00 49.07	A
MOTA	613	N	GLU		80		34.789	-17.085	38.062	1.00 45.30	A
ATOM	614	CA	GLU		80			-15.835	38.540	1.00 41.81	A
MOTA	615	CB	GLU		80		35.597	-14.850	37.405	1.00 38.87	A
ATOM	616	CG	GLU		80			-15.323	36.244	1.00 35.20	A
MOTA	617	CD	GLU		80			-14.225	35.208	1.00 36.07	· A
ATOM .	618		GLU		80			-13.744	35.000	1.00 31.43	A
ATOM	619		GLU		80			-13.828	34.607	1.00 42.76	A
ATOM	620	C	GLU		80			-15.190	39.483	1.00 42.83	A
ATOM ATOM	621	0	GLU		80			-15.440	39.393	1.00 42.30	Α
ATOM	622 623	N	SER		81			-14.358	40.390	1.00 41.48	A
ATOM	624	CA CB	SER SER		81			-13.659	41.303	1.00 40.00	A
ATOM	625	OG	SER		81 81			-13.954	42.751	1.00 39.78	A
ATOM	626	C	SER		81			-15.341 -12.188	43.031	1.00 46.97	A
ATOM	627	Ö	SER		81			-12.188	40.971	1.00 40.53	A
ATOM	628	N	LEU		82			-11.724	40.785	1.00 42.69 `	A
ATOM	629	CA	LEU		82			-10.045	40.861 40.525	1.00 38.09	A
ATOM	630	CB	LEU		82		31.792	-9.624	39.838	1.00 35.91 1.00 33.68	A
ATOM	631	CG	LEU		82		31.520	-8.125	39.671	1.00 33.68	A
MOTA	632	CD1	LEU		82		32.701	-7.380	39.073	1.00 30.29	A A
ATOM	633	CD2	LEU	Α	82	•	30.310	-7.977	38.795	1.00 37.24	A
ATOM	634	С	LEU	Α	82		33.342	-9.137	41.719	1.00 36.58	A
MOTA	635	0	LEU	Α	82		32.706	-9.282	42.774.	1.00 35.63	Ā
MOTA	636	N	PHE	A	83	,	34.282	-8.207	41.543	1.00 34.28	A
MOTA	637	CA	PHE	Α	83		34.623	-7.230	42.574	1.00 32.45	A
MOTA	638	CB	PHE	Α	83		35.901	-7.616	43.303	1.00 32.53	A.
ATOM	639	CG	PHE		83		35.726	-8.743	44.272	1.00 39.34	A
MOTA	640		PHE		83		35.694	-10.065	43.835	1.00 28.36	A
ATOM	641		PHE		83		35.546	-8.476	45.634	1.00 41.26	A
ATOM	642		PHE		83		35.482	-11.094	44.734	1.00 28.53	A
ATOM	643		PHE		83		35.334	-9.507	46.540	1.00 33.52	A
ATOM	644	CZ	PHE		83			-10.818	46.082	1.00 34.96	A
ATOM	645	G.	PHE		83		34.825	-5.872	41.928	1.00 34.82	A
ATOM	646	0	PHE		83		34.972	-5.773	40.714	1.00 38.70	A
MOTA	647	N	TRP	A	84		34.829	-4.819	42.738	1.00 33.41	A

MOTA	648	CA	TRP	A	84	35.025	-3.488	42.210	1.00 26.69	A
ATOM	649	CB	TRP	Α	84	33.738	-2.684	42.291	1.00 19.98	A
ATOM	650	CG	TRP		84	32.670	-3.249	41.424	1.00 22.79	A
ATOM	651		TRP		84	32.433	-2.955	40.037	1.00 16.75	A
MOTA	652		TRP		84	31.334	-3.733	39.626	1.00 19.29	A
ATOM	653	CE3	TRP	Α	84	33.045	-2.113	39.104	1.00 21.89	A
MOTA	654	CD1	TRP	Α	84	31.738	-4.169	41.781	1.00 22.67	A
ATOM	655	NE1	TRP	Α	84	30.925	-4.464	40.710	1.00 24.57	A
ATOM	656	CZ2	TRP	Α	84	30.831	-3.696	38.319	1.00 15.65	A
MOTA	657	CZ3			84	32.546	-2.075	37.807	1.00 14.23	A
MOTA	658	CH2			84	31.450	-2.861	37.430	1.00 16.41	A
ATOM	659	C	TRP		84	36.145	-2.755	42.904	1.00 31.00	A
MOTA	660	0	TRP		84	36.158	-2.608	44.124	1.00 34.22	A
ATOM	661	N	MET		85	37.085	-2.302	42.080	1.00 32.40	A
ATOM	662	CA	MET		85	38.274	-1.578	42.484	1.00 28.99	A
ATOM	663	CB	MET		85	39.413	-2.006	41.544	1.00 28.25	A
MOTA	664	CG	MET		85	40.702	-1.212	41.645	1.00 31.75	A
ATOM	665	SD	MET		85	41.655	-1.626	43.077	1.00 42.03	A
ATOM	666	CE	MET		85	43.040	-0.483	42.930	1.00 36.39	A
MOTA	667	C	MET		85	37.979	-0.073	42.377	1.00 29.76	A
ATOM	668	0	MET		85	37.517	0.415	41.332	1.00 28.56	A
ATOM	669	N	ASN		86	38.239	0.653	43.463	1.00 29.89	A
MOTA	670	CA	ASN		86	37.997	2.098	43.517	1.00 26.75	A
ATOM	671	CB	ASN		86	36.858	2.423	44.517	1.00 21.46	Α
ATOM	672	CG	ASN		86	35.492	1.851	44.086	1.00 31.16	Α
ATOM	673		ASN		86	35.202	0.661	44.282	1.00 29.74	A
ATOM	674		ASN		86	34.652	2.700	43.499	1.00 22.01	A
ATOM	675	C	ASN		86	39.261	2.864	43.917	1.00 26.10	A
MOTA	676	0	ASN		86	39.937	2.505	44.874	1.00 28.65	A
ATOM	677	N	VAL		87	39.566	3.925	43.181	1.00 26.23	A
ATOM	678	CA	VAL		87	40.737	4.759	43.442	1.00 21.94	A
MOTA	679	CB	VAL		87	41.826	4.557	42.354	1.00 19.79	A
ATOM	680		VAL		87	43.008	5.474	42.597	1.00 12.81	A
ATOM	681		VAL		87	42.291	3.096	42.359	1.00 14.72	A
ATOM	682	C	VAL		87	40.222	6.191	43.422	1.00 26.19	A
ATOM ATOM	683	0	VAL		87	39.786	6.717	42.390	1.00 24.87	A
ATOM	684 685	N CA	LYS		88 88	40.262	6.793	44.601	1.00 28.16	A
ATOM	686	CB	LYS		88	39.788	8.141	44.835	1.00 29.76	A
ATOM	687	CG	LYS		88	39.054	8.161	46.161	1.00 27.08	A
MOTA	688	CD	LYS		88	38.589	9.496	46.637	1.00 31.38	A
ATOM	689	CE	LYS		88	37.484 37.282	9.265 10.433	47.639 48.557	1.00 35.87	A
ATOM	690	NZ	LYS		88	36.337	10.007	49.613	1.00 34.72 1.00 43.74	A
ATOM	691	C	LYS		88	40.919	9.139	44.863	1.00 43.74	A
ATOM	692	ō	LYS		88	41.959	8.868	45.444	1.00 32.40	A
ATOM	693	N	ALA		89	40.720	10.290		1.00 40.28	A
ATOM	694	CA	ALA		89	41.741	11.326	44.216	1.00 32.42	A A
ATOM	695	CB	ALA		89	41.989	11.806	42.791	1.00 33.13	A
ATOM	696	c	ALA		89	41.262	12.477	45.085	1.00 36.67	A
ATOM	697	ō	ALA		89	40.396	13.257	44.693	1.00 36.27	A
ATOM	698	N	ILE		90	41.830	12.574	46.275	1.00 38.86	A
ATOM	699	ĊA	ILE		90	41.450	13.623	47.205	1.00 45.38	A
ATOM	700	CB	ILE		90	41.622	13.153	48.663	1.00 44.30	Ä
ATOM	701		ILE		90	41.294	14.295	49.609	1.00 40.12	A
ATOM	702		ILE		90	40.726	11.943	48.935	1.00 41.90	A
ATOM	703		ILE		90	40.723	11.323	50.303	1.00 40.34	Ā
ATOM	704	C	ILE		90	42.269	14.903	47.019	1.00 49.98	Ā
ATOM	705	ō	ILE		90	43.500	14.905	47.160	1.00 52.68	Ā
•		-		-		-5.500				

MOTA	706	N	PRO A	A 91	41.597	16.013	46.699	1.00 51.11	A
MOTA	707	CD	PRO A	4 91	40.180	16.218	46.373	1.00.51.05	A
MOTA	708	CA	PRO A	4 91	42.354	17.247	46.525	1.00 54.88	A
ATOM	709	CB	PRO A	A 91	41.354	18.160	45.836	1.00 49.07	A
ATOM	710	CG	PRO A	A 91	40.073	17.721	46.406	1.00 51.93	A
MOTA	711	С	PRO A	¥ 91	42.805	17.764	47.888	1.00 60.33	Α
MOTA	712	0	PRO A		43.021	16.988	48.812	1.00 62.83	A
MOTA	713	N	SER A	A 92	42.951	19.073	48.011	1.00 66.52	A
MOTA	714	CA	SER A	A 92	43.388	19.674	49.260	1.00 69.61	A
MOTA	715	CB	SER A	A 92	44.878	19.989	49.162	1.00 68.06	A
MOTA	716	OG	SER A	A 92	45.211	20.344	47.826	1.00 67.26	A
MOTA	717	С	SER A	A 92	42.574	20.935	49.474	1.00 73.36	A
MOTA	718	0	SER A	92	42.171	21.568	48.506	1.00 74.49	A
MOTA	719	N	MET A		42.329	21.300	50.731	1.00 79.16	· A
MOTA	720	CA	MET A	93	41.530	22.489	51.042	1.00 84.90	A
MOTA	721	CB	MET A	¥ 93	41.031	22.432	52.498	1.00 90.19	A.
MOTA	722	CG	MET A	93	39.860	23.381	52.826	1.00 98.95	A
MOTA	723	SD	MET A	93	40.266	25.089	53.357	1.00107.65	A
MOTA	724	CE	MET A	93	39.575	25.104	55.016	1.00102.52	A
MOTA	725	C	MET A	93	42.289	23.792	50.816	1.00 86.06	A
ATOM	726	0	MET A	93	43.365	23.993	51.380	1.00 85.06	A.
ATOM	727	N	ASP A	94	41.730	24.668	49.978	1.00 88.61	A
MOTA	728	CA	ASP A	94	42.347	25.963	49.708	1.00 90.81	A
MOTA	729	CB	ASP A		41.677	26.698	48.535	1.00 92.84	A
ATOM	730	CG	ASP A	94	41.750	25.936	47.221	1.00 96.92	A
MOTA	731	OD1	ASP A	94	41.812	26.599	46.158	1.00 92.90	A
ATOM	732	OD2	ASP A	94	41.725	24.686	47.243	1.00 97.61	A
MOTA	733	C	ASP A	94	42.138	26.810	50.948	1.00 91.50	A
MOTA	734	0	ASP F	94	41.001	27.036	51.360	1.00 91.94	A
ATOM	735	N	LYS A	95	43.223	27.269	51.554	1.00 92.54	Α
MOTA	736	CA	LYS A	95	43.099	28.125	52.721	1.00 93.06	Α
MOTA	737	CB	LYS A	95	44.415	28.167	53.496	1.00 92.50	Α
MOTA	738	CG	LYS A	95	44.743	26.875	54.231	1.00 91.52	A
ATOM	.739	CD	LYS A		45.179	25.761	53.302	1.00 93.56	Α
ATOM	740	CE	LYS A		46.580	26.007	52.754	1.00 93.93	Α
ATOM	741	NZ	LYS A	95	47.085	24.839	51.978	1.00 92.79	A
MOTA	742	С	LYS P		42.771	29.495	52.143	1.00 93.87	A
ATOM	743	0	LYS A		42.622	30.479	52.864	1.00 94.04	A
MOTA	744	И	SER A		42.647	29.520	50.818	1.00 95.24	A
MOTA	745	CA	SER A		42.350	30.724	50.048	1.00 95.48	Α
MOTA	746	CB	SER A		43.029	30.629	48.674	1.00 95.68	A
ATOM	747	OG	SER A		42.673	29.431	47.999	1.00 93.18	A
MOTA	748	C	SER A		40.856	31.022	49.854	1.00 94.43	A
MOTA	749	0	SER A		40.456	32.187	49.807	1.00 94.66	A
ATOM	750	N	LYS A		40.037	29.981	49.728	1.00 92.48	Α
MOTA	751	CA	LYS . F		38.602	30.173		1.00 90.51	A
MOTA	752	CB	LYS F		38.097	29.292	48.386	1.00 91.65	A
MOTA	753	CG	LYS F		38.961	29.313	47.128	1.00 94.81	A
MOTA	754	CD	LYS P		39.067	30.697	46.514	1.00 99.05	Α
MOTA	755	CE	LYS A		39.971	30. <i>6</i> 77	45.288	1.00100.93	A
MOTA	756	NZ	LYS A		40.193	32.037	44.722	1.00102.46	A
ATOM .	757	C	LYS F		37.859	29.822	50.814	1.00 87.76	A
ATOM .	758	0	LYS F		36.643	29.643	50.813	1.00 87.20	A
ATOM	759	N	LEU P		38.612	29.747	51.904	1.00 86.36	A
MOTA	760	CA	LEU A		38.102	29.402	53.228	1.00 86.15	A
ATOM	761	CB	LEU A		39.235	29.598	54.245	1.00 88.33	A
ATOM	762	CG	LEU A		39.028	29.335	55.739	1.00 89.04	A
MOTA	763	CD1	LEU A	98	38.376	30.547	56.388	1.00 86.10	A

							•				
MOTA	764	CD2	LEU	A	98		38.202	28.066	55.934	1.00 90.05	A
MOTA	765	С	LEU	A	98		36.819	30.107	53.707	1.00 85.13	A
MOTA	766	0	LEU	A	98		35.931	29.456	54.261	1.00 83.73	A
ATOM	767	N	THR	Α	99		36.719	31.423	53.510	1.00 84.73	A
ATOM	768	CA	THR	A	99		35.531	32.178	53.939	1.00 81.89	A
MOTA	769	CB	THR	A	99		35.896	33.584	54.480	1.00 83.63	A
MOTA	770	OG1	THR	Α	99		36.381	34.399	53.402	1.00 84.87	A
MOTA	771	CG2	THR	Α	99		36.965	33.490	55.572	1.00 79.10	A
ATOM	772	С	THR	Α	99		34.586	32.365	52.761	1.00 80.15	A
ATOM	773	0	THR	A	99		33.853	33.353	52.676	1.00 78.67	A
ATOM	774	N	GLU	Α	100		34.622	31.407	51.845	1.00 79.46	A
ATOM	775	CA	GLU	Α	100		33.783	31.443	50.660	1.00 77.45	A
ATOM	776	СВ	GLU				34.651	31.517	49.405	1.00 80.18	A
ATOM	777	CG	GLU	Α	100		35.286	32.873	49.165	1.00 87.28	A
ATOM	778	CD	GLU				36.285	32.850	48.025	1.00 89.03	A
ATOM	779		GLU				35.930	32.364	46.929	1.00 91.70	A
ATOM	780		GLU				37.424	33.322	48.228	1.00 92.33	A
ATOM	781	C	GLU				32.888	30.223	50.558	1.00 74.08	A
MOTA	782	ō	GLU				33.115	29.210	51.212	1.00 72.68	A
ATOM	783	N	ASN				31.856	30.341	49.736	1.00 72.40	A
ATOM	784	CA	ASN				30.943	29.240	49.499	1.00 69.74	A
ATOM	785	CB	ASN				29.596	29.774	49.040	1.00 69.70	A
ATOM	786	CG	ASN				28.633	29.938	50.185	1.00 74.66	A
ATOM	787		ASN				29.044	30.097	51.338	1.00 77.59	A
ATOM	788		ASN				27.341	29.904	49.882	1.00 74.93	A
ATOM	789	C	ASN				31.609	28.441	48.404	1.00 67.63	
ATOM	790	ō	ASN				31.759	28.924	47.280	1.00 67.83	A A
ATOM	791	N	THR				32.020	27.221	48.732	1.00 64.33	
ATOM	792	CA	THR				32.724	26.389	47.766	1.00 61.33	A
ATOM	793	CB	THR				34.200	26.260	48.153	1.00 61.33	A
ATOM	794		THR				34.296	25.666	49.453	1.00 70.60	A A
ATOM	795		THR				34.862	27.628	48.191	1.00 70.00	
ATOM	796	C	THR			•	32.194	24.982	47.556		A
ATOM	797	ō	THR				31.444	24.437	48.371	1.00 56.22	A
ATOM	798	N	LEU				32.592	24.408		1.00 51.73	A
ATOM	799	CA	LEU				32.233	23.034	46.427	1.00 55.16	A
ATOM	800	CB	LEU				31.199	22.952	46.079 44.950	1.00 52.69	A
ATOM	801	CG	LEU				31.022	21.509	44.450	1.00 48.23	A
ATOM	802		LEU				30.384	20.669		1.00 44.66	A
ATOM	803		LEU				30.164	21.476	45.562	1.00 48.29 1.00 47.17	A
ATOM	804	C	LEU				33.478	22.329	43.206 45.595		A
ATOM	805	ō	LEU				34.137		44.666	1.00 49.05	A
ATOM	806	N	GLN				33.815	22.791		1.00 47.04	A
ATOM	807	CA	GLN				34.964	21.220	46.233	1.00 48.40	A
ATOM	808	CB	GLN				36.010	20.465	45.786	1.00 46.05	A
ATOM	809	CG	GLN				37.249	20.358 21.179	46.886	1.00 48.16	A
ATOM	810	CD	GLN				38.360	20.990		1.00 49.06	A
ATOM	811		GLN				39.445	20.530	47.569	1.00 47.06 1.00 49.87	A
ATOM	812	NE2					38.099		47.410		A
ATOM	813	C	GLN					20.207	48.606	1.00 47.34	A
ATOM	814	0	GLM				34.540	19.088	45.324	1.00 44.05	A
ATOM	815		LEU				33.649	18.463	45.911	1.00 40.54	A
ATOM		N	LEU				35.163	18.631	44.249	1.00 41.40	A
	816	CA	LEU				34.863	17.319	43.729	1.00 39.84	A
ATOM ATOM	817	CB	LEU				34.625	17.383	42.230	1.00 42.67	A
	818	CG					33.441	18.223	41.760	1.00 43.19	A
MOTA	819		LEU				33.284	18.046	40.257	1.00 46.81	A
ATOM	820		LEU				32.169	17.784	42.467	1.00 49.08	A
MOTA	821	C	LEU	м	TAP		36.040	16.410	44.007	1.00 37.32	A

ATOM	822	0	LEU A	105	37.165	16.868	44.135	1.00 42.71	A
ATOM	823	N	ALA A	106	35.759	15.122	44.132	1.00 33.38	A
MOTA	824	CA	ALA A	106	36.775	14.107	44.357	1.00 28.96	2
ATOM	825	CB	ALA A	106	36.627	13.497	45.743	1.00 27.45	A
ATOM	826	C	ALA A	106	36.506	13.057	43.288	1.00 28.57	A
ATOM	827	0	ALA A		35.505	12.325	43.339	1.00 32.22	A
ATOM	828	N	ILE A		37.382	12.993	42.302	1.00 25.99	A
ATOM	829	CA	ILE A		37.195	12.040	41.228	1.00 23.30	A
ATOM	830	CB	ILE A	107	38.029	12.413	40.005	1.00 23.35	A
MOTA	831	CG2			37.535	11.621	38.791	1.00 22.54	A
MOTA	832	CG1	ILE A		37.903	13.913	39.728	1.00 19.54	A
ATOM	833	CD1	ILE A	107	36.508	14.350	39.269	1.00 19.67	A
MOTA	834	С	ILE A		37.618	10.670	41.696	1.00 24.89	A
ATOM	835	0	ILE A		38.602	10.528	42.416	1.00 27.65	A
ATOM	836	N	ILE A	108	36.872	9.658	41.278	1.00 25.44	A
MOTA	837	CA	ILE A	108	37.174	8.286	41.646	1.00 27.91	A
MOTA	838	CB	ILE A	108	36.132	7.731	42.647	1.00 29.88	A
MOTA	839	CG2	ILE A	108	36.515	6.300	43.068	1.00 16.21	A
MOTA	840	CG1	ILE A	108	36.000	8.694	43.837	1.00 24.38	A
ATOM	841	CD1	ILE A	108	34.766	8.435	44.690	1.00 17.30	A
MOTA	842	C	ILE A	108	37.101	7.435	40.391	1.00 28.20	A
ATOM	843	0	ILE A	108	36.248	7.674	39.528	1.00 26.84	A
MOTA	844	N	SER A	109	37.996	6.455	40.279	1.00 26.20	A
ATOM	845	CA	SER A	109	37.956	5.553	39.128	1.00 28.25	A
MOTA	846	CB	SER A		39.331	5.446	38.462	1.00 26.67	A
ATOM	847	OG	SER A	109	39.790	6.722	38.025	1.00 27.53	A
MOTA	848	C	SER A		37.533	4.230	39.751	1.00 28.09	A
ATOM	849	0	SER A		38.098	3.815	40.767	1.00 31.67	A
MOTA	. 850	N	ARG A	110	36.499	3.614	39.188	1.00 21.72	A
MOTA	851	CA	ARG A		35.986	2.349	39.695	1.00 25.62	A
MOTA	852	CB	ARG A	110	34.548	2.496	40.236	1.00 20.46	A
ATOM	853	CG	ARG A		33.676	1.251	39.989	1.00 24.79	A
ATOM	854	CD	ARG A		32.266	1.319	40.592	1.00 17.11	A
MOTA	855	NE	ARG A		32.356	1.368	42.041	1.00 27.71	A
MOTA	856	CZ	ARG A		31.778	0.515	42.877	1.00 25.45	A
ATOM	857		ARG A		31.031	-0.485	42.440	1.00 17.47	A
MOTA	858		ARG A		31.998	0.650	44.171	1.00 26.04	A
ATOM	859	C	ARG A		35.998	1.349	38.544	1.00 32.76	A
ATOM	860	0	ARG A		35.280	1.515	37.544	1.00 30.87	A
ATOM	861	N	ILE A		36.808	0.302	38.699	1.00 33.21	A
ATOM	862	CA	ILE A		36.924	-0.712	37.670	1.00 28.46	A
ATOM	863	CB	ILE A		38.298	-0.643	37.029	1.00 29.44	· A
ATOM	864		ILE A		38.485	0.720	36.372	1.00 25.10	A
MOTA	865 866		ILE A		39.370	-0.871	38.089	1.00 29.33	A
MOTA MOTA	867		ILE A		40.768	-0.987 -2.123	37.513 38.182	1.00 29.93	A
MOTA	868	Ċ O	ILE A		36.863	-2.123	39.359	1.00 25.36 1.00 25.09	A
MOTA	869	И	LYS A		36.305	-3.012	37.283	1.00 23.41	A
ATOM	870	CA	LYS A		36.057	-4.384	37.669	1.00 25.30	A
MOTA	871	CB	LYS A		35.390	-5.143		1.00 24.01	A
MOTA	872	CG	LYS A		34.244	-4.434	36.534 35.880	1.00 22.61	A A
MOTA	873	CD	LYS A		33.787	-5.265			
ATOM	874	CE	LYS A		32.718	-4.579	34.694 33.877	1.00 37.72 1.00 43.07	A N
MOTA	875	NZ	LYS A		32.304	-5.437	32.728	1.00 45.86	A A
MOTA	876	C	LYS A		37.358	-5.099	38.030	1.00 25.45	A
ATOM	877	ō	LYS A		38.413	-4.840	37.470	1.00 25.45	A
MOTA	878	И	LEU A		37.265	-5.995	38.990	1.00 27.32	
ATOM	879	CA	LEU A		38.393	-6.776	39.423	1.00 24.01	A A
******	012	~~			50.555	0.770	JJ. 44J	A.VU A/.TT	A

MOTA	880	CB	LEU .	A	113	38.843	-6.338	40.816	1.00	25.61	A
MOTA	881	CG	LEU .			39.787	-7.285	41.562	1.00	31.16	A
ATOM	882		LEU .		_	40.778	-7.900	40.602	1.00	43.08	A
MOTA	883	CD2	LEŲ .			40.536	-6.515 ·	42.622	1.00	33.73	A
MOTA	884	C	LEÚ .			37.847	-8.194	39.462	1.00	32.46	. A
MOTA	885	0	LEU .			36.899	-8.465	40.199	1.00	39.58	A
MOTA	886	N	TYR .	A	114	38.396	-9.091	38.644	1.00	28.70	A
MOTA	887	CA	TYR.			37.911	-10.460	38.670	1.00	29.42	A
MOTA	888	CB	TYR	A	114	37.707	-11.032	37.265		27.75	A
MOTA	889	CG	TYR .			36.707	-10.315	36.409	1.00	27.87	A
ATOM	890	CD1	TYR .			37.122	-9.570	35.308	1.00	23.04	A
ATOM	891	CE1	TYR 3			36.216	-8.902	34.522	1.00	24.87	A
MOTA	892	CD2	TYR :			35.346	-10.373	36.696	1.00	28.15	A
MOTA	893	CE2	TYR I			34.421	-9.709	35.907	1.00	29.56	A
ATOM	894	CZ	TYR I			34.863	-8.975	34.822		30.53	A
MOTA	895	OH	TYR A			33.950	-8.327	34.023	1.00	35.32	A
MOTA	896	C	TYR .				-11.362	39.398	1.00	35.05	A
ATOM	897	0	TYR I				-11.296	39.195		35.23	A
ATOM	898	N	TYR I				-12.196	40.265		37.76	A
ATOM	899	CA	TYR 2		,	-	-13.173	40.978		41.52	A
ATOM	900	CB	TYR Z				-13.488	42.319		41.85	A
ATOM	901	CG	TYR Z				-14.568	43.086		46.23	A
ATOM	902		TYR A				-14.321	43.701		49.81	A
ATOM	903	CE1	TYR Z				-15.309	44.420		50.09	Α
ATOM	904	CD2	TYR Z				-15.843	43.205		47.04	A
ATOM	905	CE2	TYR I				-16.844	43.924		48.48	A
ATOM	-	CZ	TYR A				-16.568	44.529		51.49	A
MOTA	907	OH	TYR A				-17.544	45.242		57.64	A
ATOM	908	C	TYR A				-14.359	40.034		44.16	A
MOTA	909	0	TYR A				-14.891	39.897		48.01	Α
ATOM	910	N	ARG A				-14.753	39.353		49.13	A
ATOM ATOM	911 912	CA CB	ARG A				-15.865	38.414		49.36	Α.
ATOM	913	CG	ARG A				-15.480 -16.578	37.091		52.51 55.08	A
ATOM	914	CD	ARG A				-16.578	36.030			A
ATOM	915	NE	ARG 2				-15.103	34.680		48.05	A
ATOM	916	CZ	ARG A				-14.175	34.156 33.247		50.54 48.06	A
ATOM	917		ARG A				-14.173	32.767		47.83	A A
ATOM	918		ARG A				-13.366	32.813		42.20	A
ATOM	919	C	ARG A				-17.119	38.955		51.49	Ā
ATOM	920	ō	ARG A				-17.234	38.963		52.86	A
ATOM	921	N	PRO 2				-18.078	39.421		56.20	A
ATOM	922	CD	PRO 2				-18.103	39.413		58.20	A
ATOM	923	CA	PRO 2				-19.329	39.961		62.62	A
ATOM	924	CB	PRO A				-20.198	40.121		60.18	A
ATOM	925	CG	PRO 2				-19.206			57.51	A
ATOM	926	C	PRO 2	A	117	41.287	-19.912	38.946		67.46	A
ATOM	927	0	PRO A	Ą	117	40.859	-20.413	37.916		72.30	A
ATOM	928	N	ALA A	A	118		-19.826	39.217		72.91	A
MOTA	929	CA	ALA A	A	118	43.567	-20.356	38.290		78.78	A
ATOM	930	CB ·	ALA A	Ą	118		-19.869	38.686		82.85	A
MOTA	931	C	ALA A	A	118	43.498	-21.881	38.322		79.93	A
ATOM	932	0	ALA A	A	118		-22.511	39.139		81.34	A
MOTA	933	N	LYS A			42.686	-22.461	37.434		80.10	A
ATOM	934	CA.	LYS 2	A	119	42.508	-23.913	37.360		80.33	A
ATOM	935	CB	LYS A	A	119	42.280	-24.483	38.763		82.51	A
MOTA	936	CG	LYS A	4	119	42.575	-25.970	38.913	1.00	85.21	A
ATOM	937	CD	LYS A	A	119	44.069	-26.242	39.056		85.87	A

MOTA	938	CE	LYS A	119	44.322 -27.673 39.537 1.00 89.17	A
ATOM	939	NZ	LYS A	119	45.753 -27.955 39.856 1.00 91.51	A
ATOM	940	C	LYS A	119	41.301 -24.267 36.482 1.00 79.96	A
ATOM	941	0	LYS A	119	40.769 -25.380 36.556 1.00 79.84	A
ATOM	942	N	LEU A	120	40.874 -23.323 35.650 1.00 78.20	A
MOTA	943	CA	LEU A	120	39.717 -23.538 34.786 1.00 76.07	A
ATOM	944	CB	LEU A	120	38.958 -22.223 34.611 1.00 76.08	A
MOTA	945	CG	LEU A	120	38.762 -21.423 35.904 1.00 73.67	A
MOTA	946	CD1	LEU A	120	38.028 -20.130 35.600 1.00 73.40	A
ATOM	947	CD2	LEU A	120	37.997 -22.251 36.922 1.00 72.60	A
ATOM	948	C	LEU A	120	40.116 -24.094 33.426 1.00 74.76	A
MOTA	949	0	LEU A	120	41.206 -23.817 32.923 1.00 75.67	A
ATOM	950	N	ALA A	121	39.219 ~24.875 32.832 1.00 73.89	A
ATOM	951	CA	ALA A	121	39.476 -25.495 31.534 1.00 72.13	A
ATOM	952	СВ	ALA A	121	38.502 -26.645 31.312 1.00 70.99	A
MOTA	953	C	ALA A	121	39.383 -24.512 30.378 1.00 69.72	A
ATOM	954	0	ALA A	121	40.385 -24.140 29.776 1.00 68.65	A
ATOM	955	N	LEU A	122	38.166 -24.099 30.069 1.00 69.24	A
ATOM	956	CA	LEU A	122	37.938 -23.172 28.980 1.00 70.03	A
ATOM	957	CB	LEU A	122	36.458 -22.799 28.934 1.00 66.75	A
MOTA	958	CG	LEU A	122	36.054 -21.628 28.039 1.00 67.55	A
ATOM	959	CD1	LEU A	122	36.852 -21.649 26.746 1.00 64.99	A
MOTA	960	CD2	LEU A	122	34.553 -21.701 27.779 1.00 66.80	A
MOTA	961	C	LEU A		38.788 -21.914 29.084 1.00 72.04	A
ATOM	962	0	LEU A	122	38.558 -21.076 29.946 1.00 74.93	A
ATOM	963	N	PRO A	123	39.780 -21.760 28.195 1.00 72.72	Α
MOTA	964	CD	PRO A	123	40.142 -22.671 27.094 1.00 73.51	A
ATOM	965	CA	PRO A		40.653 -20.579 28.212 1.00 73.02	A
MOTA	966	CB .	PRO A		41.753 -20.962 27.226 1.00 74.93	A '
MOTA	967	CG	PRO A		41.006 -21.783 26.211 1.00 75.79	A
ATOM	968	C	PRO A	123	39.899 -19.299 27.803 1.00 70.69	A
ATOM	969	0	PRO A	123	39.200 -19.271 26.786 1.00 70.37	A
MOTA	970	N	PRO A		40.054 -18.221 28.588 1.00 67.18	A
MOTA	971	CD	PRO A		41.089 -18.106 29.624 1.00 65.62	A
ATOM	972	CA	PRO A	124	39.411 -16.921 28.366 1.00 64.43	A
ATOM	973	CB	PRO A		40.301 -15.947 29.146 1.00 61.21	A
ATOM	974	CG	PRO A		41.563 -16.713 29.405 1.00 65.82	A
ATOM	975	C	PRO A		39.198 -16.499 26.918 1.00 65.52	A
ATOM	976	0	PRO A		38.151 -15.956 26.569 1.00 64.73	Α
ATOM	977	N	ASP A		40.185 -16.742 26.074 1.00 68.42	A
ATOM	978	CA	ASP A		40.078 -16.388 24.663 1.00 72.75	A
ATOM	979.	CB	ASP A		41.328 -16.857 23.946 1.00 79.90	A
ATOM	980	CG	ASP A		41.606 -18.324 24.204 1.00 88.64	A
ATOM	981		ASP A		40.853 -19.188 23.696 1.00 89.36	A
ATOM	982		ASP A		42.568 -18.616, 24.941 1.00 95.14	A
ATOM	983	C	ASP A		38.878 -17.081 24.024 1.00 73.33	A
ATOM	984	0	ASP A		38.199 -16.526 23.160 1.00 72.46	A
ATOM	985	N	GLN A		38.635 -18.306 24.471 1.00 73.82	A
ATOM	986	CA	GLN A		37.574 -19.158 23.957 1.00 76.31	Α
ATOM	987	CB	GLN A		38.101 -20.604 24.013 1.00 82.74	A
ATOM	988	CG	GLN A		37.267 -21.713 23.362 1.00 87.98	A
ATOM	989	CD	GLN A		37.961 -23.078 23.462 1.00 89.86	A
ATOM	990	OE1			37.348 -24.128 23.237 1.00 89.72	A
ATOM	991		GLN A		39.250 -23.060 23.799 1.00 87.56	A
ATOM	992	C	GLN A		36.239 -19.017 24.709 1.00 75.96	A
ATOM	993	0	GLN A		35.495 -19.989 24.846 1.00 78.10	A
ATOM	994	N	ALA A		35.919 -17.810 25.175 1.00 73.07	A
MOTA	995	CA	ALA A	12/	34.676 -17.602 25.925 1.00 68.39	A

MOTA	996	CB	ALA A	127	34.981	-16.896	27.235	1.00 60.93	A
ATOM	997	C	ALA A		33 555	-16.865	25.184	1.00 66.81	A
ATOM	998	ō	ALA 2			-17.283			
							25.239	1.00 66.02	A
MOTA	999	N	ALA 2	A 128	33.879	-15.776	24.495	1.00 66.13	A
ATOM	1000	CA	ALA A	A 128	32.862	-15.018	23.772	1.00 68.20	A
ATOM	1001	CB	ALA A	128	33.516	-13.901	22.974	1.00 64.84	A
ATOM	1002	C	ALA Z			-15.896	22.845	1.00 71.74	A.
MOTA	1003	0	ALA 2			-15.724	22.764	1.00 71.72	A
ATOM	1004	N	GLU A	129	32.659	-16.834	22.155	1.00 74.05	A
ATOM	1005	CA	GLU A	129	31.977	-17.737	21.227	1.00 76.20	A
ATOM	1006	CB	GLU Z			-18.739	20.643	1.00 82.11	A
MOTA	1007	CG	GLU A			-18.291	20.671	1.00 98.73	A
MOTA	1008	CD	GLU A		35.371	-19.467	20.655	1.00103.83	A
MOTA	1009	OE1	GLU A	129	36.590	-19.234	20.466	1.00106.59	A
ATOM	1010	OE2	GLU 2	129	34.911	-20.621	20.844	1.00104.99	A
ATOM	1011	C	GLU 2			-18.534	21.909	1.00 76.20	A
MOTA	1012	0	GLU A			-18.736	21.336	1.00 78.21	A
MOTA	1013	N	LYS A	1 130		-19.006	23.122	1.00 71.91	A
ATOM	1014	CA	LYS A	130	30.215	-19.813	23.888	1.00 68.25	A
ATOM	1015	CB	LYS A	130	30.865	-20.291	25.186	1.00 70.75	A
MOTA	1016	CG	LYS 2			-21.020	25.004	1.00 74.67	A
ATOM	1017	CD	LYS A			-22.386	24.366	1.00 74.27	A
MOTA	1018	CE	LYS 2			-23.059	24.080	1.00 73.75	A
MOTA	1019	NZ	LYS A	130	33.149	-24.415	23.484	1.00 73.72	A
MOTA	1020	C	LYS 2	130	28.933	-19.071	24.224	1.00 68.00	A
ATOM	1021	Ö.	LYS A			-19.644	24.827	1.00 67.92	A
ATOM	1022	N	LEU A			-17.802	23.830	1.00 67.34	A
MOTA	1023	CA	LEU A		27.680	-16.992	24.118	1.00 67.92	A
MOTA	1024	CB	LEU A	131	28.002	-15.506	23.974	1.00 64.70	A
ATOM	1025	CG	LEU A	131	26.852	-14.610	24.457	1.00 60.80	A
MOTA	1026		LEU A			-14.706	25.984	1.00 54.51	A
			LEU A						
MOTA	1027					-13.177	24.027	1.00 54.96	A
MOTA	1028	C	LEU A		26.484	-17.299	23.242	1.00 72.16	A
MOTA	1029	0	LEU A	131	26.469	-16.941	22.065	1.00 76.77	A
ATOM	1030	N	ARG A	132	25.473	-17.939	23.816	1.00 75.27	A
ATOM	1031	CA	ARG A	132		-18.262	23.065	1.00 81.32	A
ATOM	1032	CB	ARG A			-19.650		1.00 85.77	
							23.456		A
ATOM	1033	CG	ARG A			-20.748	23.318	1.00 94.11	A
ATOM	1034	CD	ARG A	132	24.400	-22.004	24.091	1.00 98.71	A
ATOM	1035	NE	ARG A	132	25.538	-22.878	24.380	1.00103.00	A
MOTA	1036	CZ	ARG A	132	25.499	-23.918	25.212	1.00103.86	A
MOTA	1037		ARG 2			-24.229	25.847	1.00101.67	A
					•	•			
MOTA	1038		ARG A			-24.639	25.421	1.00104.18	A
MOTA	1039	C	ARG A			-17.208	23.368	1.00 82.53	A
MOTA	1040	0	ARG A	132	23.477	-16.217	24.044	1.00 80.66	Α
ATOM	1041	N	PHE A	133	21.987	-17.414	22.868	1.00 85.49	A
ATOM	1042	CA	PHE 2			-16.460	23.101	1.00 89.99	A
			PHE A						
ATOM	1043	CB				-15.460	21.947	1.00 89.83	A
MOTA	1044	CG	PHE A		22.019	-14.545	21.863	1.00 89.92	A
ATOM	1045	CD1	PHE A	133	23.251	-15.019	21.431	1.00 89.46	A
MOTA	1046	CD2	PHE A	133	21.907	-13.210	22.242	1.00 90.61	· A
ATOM	1047		PHE A			-14.180	21.379	1.00 91.51	A
ATOM	1048		PHE A			-12.358	22.195	1.00 89.22	A
MOTA	1049	cz	PHE A			-12.843	21.762	1.00 90.80	A
MOTA	1050	С	PHE A	133	19.523	-17.070	23.319	1.00 93.54	A
ATOM	1051	0	PHE A	133		-18.258	23.612	1.00 95.64	A
ATOM	1052	N	ARG A			-16.222	23.177	1.00 95.33	A
MOTA	1053	CA	ARG A	1 134	1/.110	-16.591	23.342	1.00 98.47	A

MOTA	1054	CB	ARG A	134	16.836 -17	.049	24.770	1.00 96.46	A
MOTA	1055	CG	ARG A	134	15.363 -17	.236	25.084	1.00 96.89	A
ATOM	1056	CD	ARG A	134	15.143 -17	.231	26.586	1.00 99.77	A
MOTA	1057	NE	ARG A	134	15.884 -18	.301	27.247	1.00103.07	A
ATOM	1058	CZ	ARG A	134	16.197 -18	.302	28.539	1.00103.43	A
MOTA	1059	NH1			15.836 -17		29.312	1.00102.01	A
ATOM	1060	NH2			16.869 -19		29.061	1.00102.06	A
ATOM	1061	С	ARG A		16.351 -15		23.065	1.00101.77	
ATOM	1062	ō	ARG A		16.078 -14		23.979		A
ATOM	1063	N	ARG A		16.006 -15		21.799	1.00102.68	A
ATOM	1064	CA	ARG A		15.332 -13		21.799	1.00103.79	A
ATOM	1065	CB	ARG A		16.003 -13			1.00104.26	A
ATOM	1066		ARG A				20.147	1.00104.33	A
		CG			15.770 -14		18.904	1.00101.69	A
ATOM	1067	CD	ARG A		14.953 -13		17.948	1.00103.33	A
ATOM	1068	NE	ARG A		15.578 -12		17.768	1.00102.02	A
ATOM	1069	CZ	ARG A		14.944 -10		17.337	1.00103.23	. А
ATOM	1070		ARG A			.799	17.208	1.00103.92	A
ATOM	1071		ARG A		13.651 ~10		17.044	1.00103.58	A
ATOM	1072	C	ARG A		13.832 -13		21.173	1.00104.63	A
ATOM	1073	0	ARG A		13.367 -14		20.267	1.00105.45	A
MOTA	1074	N	SER A		13.081 -13	.204	22.000	1.00104.76	A
MOTA	1075	CA	SER A		11.627 -13	.140	21.874	1.00106.02	A
ATOM	1076	CB	SER A	136	10.964 -13	.037	23.254	1.00104.91	·A
ATOM	1077	OG	SER A		11.050 -14	.261	23.963	1.00104.33	А
ATOM	1078	C	SER A	136	11.301 -11	.895	21.045	1.00107.69	A
ATOM	1079	0	SER A	136	11.995 -11	.591	20.071	1.00108.16	A
ATOM	1080	N	ALA A	137	10.248 -11	.179	21.424	1.00107.96	A
MOTA	1081	CA	ALA A	137	9.859 -9	.962	20.719	1.00108.16	A
MOTA	1082	CB	ALA A	137	8.419 -10	.067	20.242	1.00107.11	A
MOTA	1083	C	ALA A			.801	21.695	1.00108.96	A
MOTA	1084	0	ALA A	137		.688	21.444	1.00109.33	A
MOTA	1085	N	ASN A	138		.083	22.811	1.00108.20	A
ATOM	1086	CA	ASN A	138		.099	23.861	1.00106.68	A
ATOM	1087	CB	ASN A			.772	24.554	1.00107.71	A
ATOM	1088	CG	ASN A			.019	24.898	1.00107.21	A
ATOM	1089		ASN A			.931	25.595	1.00103.20	A
ATOM	1090		ASN A			.058	24.408	1.00104.18	A
MOTA	1091	C	ASN A			.551	24.912	1.00104.33	A
ATOM	1092	0	ASN A			.729	25.639	1.00102.13	A
ATOM	1093	N	SER A			.853	24.982	1.00103.36	Ā
ATOM	1094	CA	SER A		13.066 -10		25.993	1.00101.80	A
ATOM	1095	CB	SER A		12.255 -11		27.041	1.00101.56	A
ATOM	1096	OG	SER A		11.137 -10		27.470	1.00102.16	A
ATOM	1097	c	SER A		14.228 -11		25.504	1.00102.10	Ā
ATOM	1098	ō	SER A		14.211 -12		25.672	1.00100.27	Ā
ATOM	1099	N	LEU A		15.237 -10		24.906	1.00100.30	Ā
ATOM	1100	CA	LEU A		16.422 -11		24.434	1.00 97.34	
ATOM	1101	CB	LEU A		17.234 -10		23.496	1.00 91.63	A
ATOM	1102	CG	LEU A		18.335 -11		22.696		A
ATOM	1102		LEU A					1.00 93.83	A
					19.083 -10		21.856	1.00 92.02	A
ATOM	1104		LEU A		19.286 -11		23.637	1.00 93.87	A
MOTA	1105	C	LEU A		17.246 -11		25.683	1.00 89.12	A
ATOM	1106	0	LEU A		17.584 -10		26.450	1.00 91.60	A
ATOM	1107	N	THR A		17.590 -12		25.880	1.00 84.11	A
ATOM	1108	CA	THR A		18.323 -13		27.074	1.00 81.12	A
ATOM	1109	CB	THR A		17.502 -14		27.881	1.00 80.24	A
ATOM	1110		THR A		16.219 -13		28.197	1.00. 77.38	A
ATOM	1111	CG2	THR A	141	18.225 -14	.717	29.179	1.00 80.24	A

MOTA	1112	C	THR A	141	19.741	-13.824	26.870	1.00 80.24	A
MOTA	1113	0	THR A	141	19.933	-15.027	26.658	1.00 79.58	A
MOTA	1114	N	LEU A	142	20.729	-12.931	26.957	1.00 76.82	A
ATOM	1115	CA	LEU P	142	22.134	-13.318	26.815	1.00 72.84	A
MOTA	1116	CB	LEU A	142	23.061	-12.165	27.216	1.00 68.91	A
MOTA	1117	CG	LEU A	142	23.045	-10.770	26.562	1.00 71.48	A
MOTA	1118	CD1	LEU A	142	23.732	-10.801	25.214	1.00 66.22	A
MOTA	1119	CD2	LEU F	142	21.617	-10.252	26.449	1.00 66.28	A
ATOM	1120	С	LEU A	142	22.357	-14.496	27.766	1.00 71.91	A
MOTA	1121	0	LEU A			-14.464	28.915	1.00 71.08	A
ATOM	1122	N	ILE A	143	23.022	-15.538	27.288	1.00 71.51	A
MOTA	1123	CA	ILE A			-16.709	28.119	1.00 70.41	A
ATOM	1124	CB	ILE A	143		-17.881	27.683	1.00 70.24	A
ATOM	1125	CG2	ILE A	143	22.132	-17.817	26.195	1.00 71.96	A
ATOM	1126		ILE A		22.972	-19.223	28.096	1.00 69.66	A
MOTA	1127	CD1	ILE A	143		-19.457	29.592	1.00 74.41	A
ATOM	1128	C	ILE A			-17.131	28.063	1.00 70.37	A
MOTA	1129	0	ILE A			-17.500	27.010	1.00 72.24	A
ATOM	1130	N	ASN A			-17.076	29.214	1.00 69.73	A
ATOM	1131	CA	ASN A			-17.429	29.323	1.00 67.88	A
ATOM	1132	CB	ASN A			-16.225	29.855	1.00 65.44	A
ATOM	1133	CG	ASN A			-16.559	30.196	1.00 65.15	A
ATOM	1134		ASN A			-17.629	29.853	1.00 62.67	A
ATOM	1135		ASN A			-15.630	30.868	1.00 63.84	A
ATOM	1136	C	ASN A			-18.645	30.221	1.00 66.60	A
ATOM	1137	ō	ASN A			-18.591	31.425	1.00 66.49	A
ATOM	1138	N	PRO A			-19.765	29.631	1.00 66.80	A
ATOM	1139	CD	PRO A			-19.968	28.167	1.00 67.42	A
ATOM	1140	CA	PRO A			-21.032	30.321	1.00 65.43	Ā
ATOM	1141	CB	PRO A		27.378		29.274	1.00 64.83	A
ATOM	1142	CG	PRO A			-21.411	28.025	1.00 67.40	A
ATOM	1143	C	PRO A			-21.203	30.774	1.00 65.99	A
ATOM	1144	Ö	PRO A			-22.140	31.506	1.00 68.84	A
ATOM	1145	N	THR A			-20.307	30.332	1.00 64.37	A
ATOM	1146	CA	THR A			-20.374	30.532	1.00 61.20	A
ATOM	1147	CB	THR A			-19.421	29.813	1.00 60.13	A
ATOM	1148		THR A			-18.152	30.461	1.00 48.37	A
ATOM	1149		THR A			-19.221	28.472	1.00 58.08	
ATOM	1150	C	THR A			-19.958	32.144	1.00 63.71	A A
ATOM	1151	Õ	THR A			-19.755	32.851	1.00 68.20	
ATOM	1152	N	PRO A			-19.850	32.621	1.00 63.27	A A
ATOM	1153	CD	PRO A			-20.642	32.171	1.00 65.51	A
ATOM	1154	CA	PRO A			-19.440	34.015	1.00 60.71	
ATOM	1155	CB	PRO A			-20.482	34.538	1.00 63.94	A A
ATOM	1156	CG	PRO A			-20.596	33.384	1.00 65.82	A
ATOM	1157	C	PRO A			-18.034	34.114	1.00 58.31	
MOTA	1158	Ö	PRO A			-17.691	35.111	1.00 59.00	A
MOTA	1159	N		148		-17.230	33.076	1.00 55.78	A
MOTA	1160	CA	TYR A			-15.860	33.076	1.00 54.68	A
ATOM	1161	CB	TYR A			-15.657			A
ATOM	1162	CG	TYR A				31.915	1.00 52.42	A
	1163					-16.669	31.835	1.00 54.53	A
MOTA MOTA	1164	CDI	TYR A	1/0		-17.945	31.314	1.00 53.25	A
						-18.882	31:249	1.00 52.08	A
MOTA	1165		TYR A			-16.355	32.286	1.00 59.18	A
MOTA	1166		TYR A			-17.287	32.227	1.00 57.18	A
MOTA	1167	CZ	TYR A			-18.545	31.712	1.00 56.02	A
ATOM	1168	OH	TYR A			-19.464	31.703	1.00 60.53	A
MOTA	1169	С	TYR A	. 148	32.891	-14.826	32.865	1.00 52.36	A

MOTA	1170	0	TYR A	148	31.875	-15.091	32.218	1.00 54.15	A
MOTA	1171	N	TYR A	149	33.096	-13.636	33.412	1.00 46.88	A
MOTA	1172	CA	TYR A	149	32.109	-12.589	33.232	1.00 45.19	Α
MOTA	1173	CB	TYR A			-11.433	.34.219	1.00 43.03	A
MOTA	1174	CG	TYR A			-11.614	35.559	1.00 42.11	А
MOTA	1175	CD1			32.240	-12.391	36.556	1.00 41.82	A
MOTA	1176	CE1	TYR A	149		-12.596	37.779	1.00 43.09	A
MOTA	1177	CD2	TYR A	•	30.420	-11.040	35.814	1.00 45.78	A
MOTA	1178	CE2	TYR A	149		-11.242	37.037	1.00 40.20	A
MOTA	1179	CZ	TYR A	149		-12.017	38.011	1.00 39.11	A
MOTA	1180	OH	TYR A			-12.203	39.219	1.00 39.29	A
MOTA	1181	C	TYR A	149	32.218	-12.086	31.793	1.00 42.46	A
MOTA	1182	0	TYR A	149		-11.712	31.333	1.00 43.49	Α
MOTA	1183	N	LEU A	150	31.108	-12.083	31.074	1.00 38.24	A
MOTA	1184	CA	LEU A	150	31.152	-11.615	29.709	1.00 38.20	A
ATOM	1185	CB	LEU A			-12.528	28.793	1.00 41.63	. A
MOTA	1186	CG	LEU A			-13.982	28.638	1.00 47.76	A
ATOM	1187		LEU A			-14.693	27.628	1.00 49.37	A
ATOM	1188	CD2	LEU A		32.260	-14.027	28.168	1.00 46.98	A
ATOM	1189	C	LEU A			-10.190	29.624	1.00 37.43	A
MOTA	1190	0	LEU A		29.509	-9.886	29.957	1.00 38.19	A
MOTA	1191	N	THR A		31.538	-9.305	29.186	1.00 37.68	Α
ATOM	1192	CA	THR A		31.159	-7.918	29.033	1.00 39.56	A
MOTA	1193	CB	THR A		32.329	-6.956	29.381	1.00 37.50	, A
MOTA	1194	OG1	THR A		32.765	-7.189	30.725	1.00 33.72	A
MOTA	1195		THR A		31.878	-5.504	29.273	1.00 36.25	A
ATOM	1196	C	THR A		30.735	-7.741	27.579	1.00 43.30	A
ATOM	1197	0	THR A		31.529	-7.346	26.726	1.00 45.62	A
ATOM	1198	N	VAL A		29.477	-8.069	27.308	1.00 46.36	A
ATOM	1199	CA	VAL A		28.908	-7.953	25.973	1.00 50.28	Α
ATOM	1200	CB	VAL A		27.574	-8.721	25.865	1.00 54.87	Α
MOTA	1201		VAL A		26.896	-8.402	24.544	1.00 53.66	Α
ATOM	1202		VAL A		27.820		25.989	1.00 53.64	A
MOTA	1203	C	VAL A		28.635	-6.503	25.633	1.00 51.96	A
MOTA	1204	0	VAL A		27.900	-5.829	26.337	1.00 54.79	A
MOTA	1205	N	THR A		29.232	-6.033	24.548	1.00 55.97	A
ATOM	1206	CA	THR A		29.048	-4.662	24.096	1.00 58.87	A
MOTA	1207	CB	THR A		30.305	-3.816	24.398	1.00 58.83	A
MOTA	1208	OG1			30.090	-2.452	24.002	1.00 59.83	A
ATOM	1209	CG2			31.514	-4.391	23.667	1.00 56.99	A
ATOM	1210	C	THR A		28.764	-4.688	22.584	1.00 64.16	A
ATOM	1211	0	THR A		28.926	-5.728	21.927	1.00 63.27	A
MOTA	1212	И	GLU A		28.336	-3.547	22.042	1.00 68.30	A
ATOM	1213	CA	GLU A		27.997	-3.419	20.621	1.00 69.78	A
ATOM	1214	CB	GLU A		29.257	-3.406	19.759	1.00 67.91	A
ATOM	1215 1216	CG	GLU A		30.100	-2.168	19.957	1.00 74.41	A
ATOM	1216	CD			31.049	-1.918	18.803	1.00 80.81	A
MOTA		OE1	GLU A		31.805	-0.919	18.846	1.00 81.08	A
ATOM	1218		GLU A		31.031	-2.721	17.847	1.00 87.45	A
MOTA	1219 1220	C	GLU A		27.064 27.249	-4.532	20.161	1.00 70.72	A
MOTA		0				-5.118	19.097	1.00 73.11	A
MOTA	1221	N	LEU A		26.058	-4.816	20.979	1.00 72.02 1.00 73.50	A
MOTA	1222	CA	LEU A		25.078	-5.850	20.678		A
MOTA	1223	CB	LEU A		24.353 23.396	-6.279	21.955	1.00 65.70 1.00 60.65	A
MOTA	1224	CG				-7.462	21.844	1.00 60.65	A A
MOTA	1225	CD1	LEU A		24.187 22.649	-8.721 -7.642	21.509 23.149		A
MOTA	1226		LEU A			-7.642 -5.277	19.695	1.00 58.58	A A
MOTA	1227	С	пео А	. 155	24.072	-5.277	T3.032	1.00 79.03	A

ATOM	1228	0	LEU A	155	23.751	-4.091	19.754	1.00 79.45	A
MOTA	· 1229	N	ASN A	156	23.573	-6.116	18.793	1.00 85.28	A
MOTA	1230	CA	ASN A	156	22.603	-5.662	17.804	1.00 88.93	A
MOTA	1231	CB	ASN A	156	23.339	-5.108	16.594	1.00 87.25	A
ATOM	1232	CG	ASN A	156	24.418	-4.130	16.988	1.00 89.36	A
MOTA	1233	OD1	ASN A	156	24.134	-3.059	17.524	1.00 89.06	A
MOTA	1234	ND2	ASN A	156	25.670	-4.500	16.746	1.00 90.53	A
MOTA	1235	C	ASN A	156	21.653	-6.765	17.374	1.00 91.63	A
MOTA	1236	0	ASN A	156	22.066	-7.907	17.158	1.00 89.76	A
MOTA	1237	N	ALA A	157	20.374	-6.414	17.267	1.00 96.18	A
ATOM	1238	CA	ALA A	157	19.337	-7.354	16.851	1.00 99.74	A
MOTA	1239	CB	ALA A	157	17.969	-6.847	17.283	1.00100.77	A
MOTA	1240	C	ALA A	157	19.404	-7.455	15.334	1.00102.40	A
MOTA	1241	0	ALA A	157	18.387	-7.632	14.659	1.00103.36	Α
MOTA	1242	N	GLY A	158	20.622	-7.332	14.816	1.00105.21	A
MOTA	1243	CA	GLY. A	158	20.850	-7.392	13.387	1.00106.57	A
ATOM	1244	C	GLY A	158	21.156	-6.006	12.858	1.00107.97	A
MOTA.	1245	0	GLY A	158	22.228	-5.770	12.299	1.00108.06	A
MOTA	1246	N	THR A	159	20.206	-5.093	13.044	1.00109.17	A
ATOM	1247	CA	THR A	159	20.343	-3.712	12.592	1.00111.28	A
MOTA	1248	CB	THR A		19.239	-3.331	11.594	1.00112.70	A
MOTA	1249	OG1	THR A	159	17.965	-3.416	12.247	1.00116.55	A
MOTA	1250	CG2			19.248	-4.268	10.395	1.00115.55	A
MOTA	1251	C	THR A	159	20.196	-2.802	13.795	1.00111.85	A
MOTA	1252	0	THR A	159	20.968	-1.860	13.978	1.00112.27	A
MOTA	1253	N	ARG A		19.187	-3.096	14.608	1.00112.10	A
MOTA	1254	CA	ARG A		18.912	-2.321	15.804	1.00113.25	A
MOTA	1255	CB	ARG A		17.617	-2.813	16.458	1.00118.41	. A
ATOM	1256	CG	ARG A	160	17.133	-1.969	17.637	1.00125.82	A
MOTA	1257	CD	ARG A		16.451	-0.677	17.169	1.00131.90	A
MOTA	1258	NE	ARG A		15.752	0.009	18.255	1.00136.67	· A
MOTA	1259	CZ	ARG A	160	16.332	0.811	19.144	1.00137.21	A
ATOM	1260		ARG A		17.637	1.050	19.083	1.00138.96.	A
MOTA	1261		ARG A	160	15.606	1.352	20.116	1.00136.47	A
ATOM	1262	C	ARG A		20.069	-2.472	16.783	1.00111.18	A
ATOM	1263	0	ARG A		20.605	-3.568	16.967	1.00110.16	A
MOTA	1264	N	VAL A	161	20.459	-1.362	17.400	1.00108.44	A
ATOM	1265	CA	VAL A		21.540	-1.371	18.378	1.00105.90	A
ATOM	1266	CB	VAL A		22.426	-0.108	18.250	1.00108.81	A
MOTA	1267		VAL A		21.584	1.151	18.459	1.00109.63	A
ATOM	1268		VAL A		23.573	-0.172	19.255	1.00107.85	A
MOTA	1269	C	VAL A		20.942	-1.429	19.782	1.00101.78	· A
MOTA	1270	0	VAL A		20.040	-0.658	20.120	1.00101.40	A
MOTA	1271	N	LEU A		21.445	-2.343	20.602	1.00 97.13	A
ATOM	1272	CA	LEU A		20.930	-2.488	21.957	1.00 93.47	A
MOTA	1273	CB	LEU A		20.695	-3.967	22.263	1.00 93.19	A
MOTA	1274	CG	LEU A		19.669	-4.649	21.364	1.00 92.83	A
MOTA	1275		LEU A		19.474	-6.093	21.809	1.00 92.94	A
ATOM	1276		LEU A		18.361	-3.880	21.436	1.00 91.31	A
ATOM	1277	C	LEU A		21.804	-1.878	23.052	1.00 89.80	A
ATOM	1278	0	LEU A		22.695	-1.061	22.795	1.00 88.59	A
ATOM	1279	N	GLU A		21.529	-2.286	24.284	1.00 85.62	A
MOTA	1280	CA	GLU A		22.263	-1.798	25.437	1.00 80.86	Α
ATOM	1281	CB	GLU A		21.273	-1.389	26.525	1.00 84.16	A
MOTA	1282	· CG	GLU A		21.866	-0.544	27.633	1.00 89.10	A
MOTA	1283	CD	GLU A		20.838	0.383	28.250	1.00 90.24	Α
ATOM	1284		GLU A		20.485	1.389	27.595	1.00 90.20	A
ATOM	1285	OE2	GLU A	163	20.376	0.102	29.379	1.00 92.14	A

MOTA	1286	C	GLU	A 163	23.217	7 -2.881	25.943	1.00 75.63	A
ATOM	1287			A 163	22.84			1.00 74.97	
		0					26.051		A
ATOM	1288	N	ASN	A 164	24.449	-2.469	26.239	1.00 67.82	A
MOTA	1289	CA	ASN	A 164	25.494	-3.371	26.715	1.00 60.23	A
	1290								
ATOM		CB		A 164	26.691		27.183	1.00 61.03	A
MOTA	1291	CG	ASN	A 164	27.091	L -1.509	26.187	1.00 65.34	Α
ATOM	1292	נתם	ASM	A 164	27.592	-1.816	25.104	1.00 67.49	A
_									
ATOM	1293	ND2		A 164	. 26.858	3 -0.251	26.538	1.00 72.33	A
ATOM	1294	С	ASN	A 164	25.036	-4.273	27.843	1.00 56.85	A
MOTA	1295	0		A 164	24.095		28.564	1.00 60.38	A
ATOM	1296	N	ALA	A 165	25.709	-5.399	28.009	1.00 52.80	Α
ATOM	1297	CA	ALA	A 165	25.332	-6.316	29.065	1.00 51.59	A
MOTA	1298	CB		A 165	24.400		28.527	1.00 55.00	A
ATOM	1299	C	ALA	A 165	26.550	-6.964	29.682	1.00 52.66	A
ATOM	1300	0	ALA	A 165	27.608	3 -7.063	29.057	1.00 52.84	A
MOTA	1301	N		A 166	26.387		30.930	1.00 50.08	A
ATOM	1302	CA	ΓEU	A 166	27.442	-8.042	31.677	1.00 46.09	A
ATOM	1303	CB	LEU	A 166	27.784	-7.239	32.930	1.00 39.06	A
MOTA	1304	CG		A 166	28.805		33.879	1.00 44.53	A
ATOM	1305			A 166	30.155	-8.052	33.160	1.00 36.48	A
ATOM	1306	CD2	LEU	A 166	28.968	6.997	35.109	1.00 32.66	A
MOTA	1307	C		A 166	26.849	-9.382	32.050	1.00 45.68	A
MOTA	1308	0		A 166	25.994		32.921	1.00 47.46	Α
MOTA	1309	N	VAL	A 167	27.289	-10.438	31.381	1.00 46.23	A
ATOM	1310	CA	VAL	A 167	26.726	-11.744	31.667	1.00 46.03	A
ATOM	1311	CB		A 167		-12.542	30.396	1.00 46.87	A
MOTA	1312	CGI	VAL.	A 167	25.648	3 -13.784	30.749	1.00 48.77	A
MOTA	1313	CG2	VAL	A 167	25.683	-11.675	29.393	1.00 48.21	A
ATOM	1314	C	VAT.	A 167	27 588	-12.581	32.568	1.00 46.09	Α
ATOM	1315	0		A 167		-13.013	32.191	1.00 48.22	A
ATOM	1316	N	PRO .	A 168	27.093	-12.836	33.780	1.00 47.27	A
MOTA	1317	CD	PRO	A 168	25.763	-12.376	34.217	1.00 46.22	A
		CA							
MOTA	1318			A 168		-13.620	34.829	1.00 49.84	A
ATOM	1319	CB	PRO	A 168	26.731	13.552	35.968	1.00 51.34	A
ATOM	1320	CG	PRO	A 168	25.408	-13.408	35.241	1.00 48.56	A
MOTA	1321	C		A 168		-15.055	34.442		A
ATOM	1322	0	PRO	A 168	27.392	-15.656	33.617	1.00 54.95	A
ATOM	1323	N	PRO .	A 169	29.122	-15.624	35.048	1.00 56.08	A
MOTA	1324	CD	PRO	A 169	30.000	-14.946	36.017	1.00 58.84	A
ATOM	1325	CA		A 169		-16.993	34.808	1.00 58.16	Α
MOTA	1326	CB	PRO	A 169	30.693	-17.168	35.849	1.00 58.15	A
MOTA	1327	CG	PRO .	A 169	31.251	15.804	35.967	1.00 61.56	A
ATOM	1328	C	DP∩	A 169		-17.995	35.025	1.00 58.07	A
ATOM	1329	0		A 169	27.704	-17.871	35.981	1.00 59.45	A
MOTA	1330	N	MET	A 170	28.368	-18.987	34.147	1.00 57.55	A
ATOM	1331	CA		A 170	27 225	-20.002	34.273	1.00 53.80	A
MOTA	1332	CB		A 170		-21.032	35.303	1.00 53.82	A
MOTA	1333	CG	MET	A 170	28.948	-21.857	34.811	1.00 67.88	A
ATOM	1334	SD	MET	A 170	29.786	-22.829	36.069	1.00 79.30	A
MOTA	1335	CE		A 170		-21.887	36.209	1.00 77.73	A
MOTA	1336	C	\mathtt{MET}	A 170	26.009	-19.369	34.673	1.00 52.55	A
ATOM	1337	0	MET	A 170	25.255	-19.924	35.477	1.00 50.48	A
ATOM	1338	Ŋ		A 171		-18.194	34.107	1.00 49.32	A
MOTA	1339	CA		A 171		1 -17.481	34.394	1.00 51.25	A
MOTA	1340	С	GLY	A 171	23.985	-16.844	33.134	1.00 57.47	A
MOTA	1341	0		A 171		-17.222	32.030	1.00 59.54	A
MOTA	1342	N		A 172		-15.869	33.289	1.00 60.67	A
MOTA	1343	CA	GLU .	A 172	22.500	-15.206	32.141	1.00 64.80	Α

ATOM	1344	CB	GLU A	172	21.456	-16.129	31.516	1.00 71.05	A
ATOM	1345	CG	GLU A	172	20.494	-16.737	32.526	1.00 78.57	A
ATOM	1346	CD	GLU A	172	19.669	-17.861	31.931	1.00 83.92	A
MOTA	1347	OE1				-17.588	31.004	1.00 84.47	A
ATOM	1348	OE2	GLU A	172		-19.019	32.387	1.00 86.75	A
ATOM	1349	C	GLU A			-13.863	32.481	1.00 64.91	A
ATOM	1350	ō	GLU A			-13.562	33.635	1.00 67.26	A
ATOM	1351	N	SER A			-13.063	31.453	1.00 66.61	A
ATOM	1352	CA	SER A			-11.741	31.612	1.00 69.38	A
ATOM	1353	ĊB	SER A			-10.690	31.610	1.00 68.94	A
ATOM	1354	OG	SER A			-11.206	32.208	1.00 58.34	A
ATOM	1355	C	SER A			-11.482		1.00 74.42	
ATOM	1356	0	SER A	. –		-11.944	30.440 29.325	1.00 71.97	A
ATOM			ALA A						A
	1357	N	ALA A			-10.742 -10.442	30.684	1.00 75.48	A
MOTA MOTA	1358	CA					29.622	1.00 78.56	A
	1359	CB	ALA A			-10.921	30.018	1.00 77.27	A
ATOM	1360	C	ALA A		18.063	-8.952	29.289	1.00 81.26	A
ATOM	1361	0	ALA A		17.719	-8.127	30.136	1.00 83.51	A
ATOM:	1362	N	VAL A		18.444	-8.611	28.064	1.00 83.71	A
ATOM	1363	CA	VAL A		18.407	-7.230	27.608	1.00 90.85	A
ATOM	1364	CB	VAL A		19.557	-6.926	26.622	1.00 92.75	A
ATOM	1365		VAL A		19.324	-5.570	25.946	1.00 87.47	A
MOTA	1366		VAL A		20.900	-6.936	27.336	1.00 93.36	A
ATOM	1367	C	VAL A		17.079	-7.025	26.890	1.00 96.22	A
ATOM	1368	0	VAL A		16.670	-7.869	26.094	1.00 97.56	A
ATOM	1369	N	LYS A		16.406	-5.915	27.188	1.00 99.57	. A
ATOM .	1370	CA	LYS A	176	15.111	-5.630	26.573	1.00103.13	Α
ATOM	1371	CB	LYS A		14.599	-4.241	26.970	1.00101.70	A
MOTA	1372	CG	LYS A	176	14.200	-4.103	28.450	1.00104.25	Α
ATOM	1373	CD	LYS A	176	15.409	-4.184	29.395	1.00100.55	A
MOTA	1374	CE	LYS A	176	15.046	-3.771	30.825	1.00 93.06	A
ATOM	1375	NZ	LYS A	176	13.964	-4.622	31.397	1.00 86.44	A
ATOM	1376	C	LYS A	176	15.210	-5.711	25.048	1.00107.60	A
ATOM	1377	0	LYS A	176	15.921	-4.928	24.417	1.00108.29	A
ATOM	1378	N	LEU A	177	14.496	-6.673	24.464	1.00110.94	A
ATOM	1379	CA	LEU A	177	14.457	-6.886	23.016	1.00114.23	A
ATOM	1380	CB	LEU A	177	14.101	-8.349	22.756	1.00110.63	A
ATOM	1381	CG	LEU A	1.77	14.158	-8.910	21.333	1.00108.29	A
ATOM	1382	CD1			15.327	-8.307	20.553	1.00106.45	A
ATOM	1383	CD2				-10.432	21.404	1.00106.48	A
ATOM	1384	C	LEU A		13.420	-5.929	22.402	1.00118.01	A
MOTA	1385	Ō	LEU A		12.214	-6.091	22.592	1.00117.68	A
ATOM	1386	N	PRO A		13.894	-4.926	21.642	1.00121.47	· A
ATOM	1387	CD	PRO A		15.313	-4.810	21.255	1.00122.27	A
ATOM	1388	CA	PRO A		13.107	-3.885	20.971	1.00124.48	A
ATOM	1389	CB	PRO A		14.183	-2.987	20.376	1.00122.83	A
ATOM	1390	CG	PRO A		15.233	-3.964	20.001	1.00124.50	A
ATOM	1391	C	PRO A		12.074	-4.289	19.922	1.00124.00	A
ATOM	1392	Õ	PRO A		11.162	-3.513	19.622	1.00120.02	A
ATOM	1393	N	SER A		12.215	-5.485	19.358	1.00129.47	
						-5.485	18.318		A N
MOTA	1394	CA	SER A		11.303			1.00132.08	A
MOTA	1395	CB	SER A		9.832	-5.742	18.705	1.00132.69	A
MOTA	1396	OG	SER A		8.953	-6.444	17.839	1.00133.48	A
ATOM	1397	C	SER A		11.598	-5.436	16.910	1.00132.03	A
MOTA	1398	0	SER A		11.094	-5.964	15.905	1.00131.83	A
MOTA	1399	N	ASP A		12.398	-4.368	16.846	1.00131.38	A
ATOM	1400	CA	ASP A		12.847	-3.787	15.568	1.00129.15	A
ATOM	1401	CB	ASP A	180	13.446	-2.385	15.784	1.00129.31	A

MOTA	1402	CG	ASP A	180	12.441	-1.388	16.322	1.00129.01	A
MOTA	1403	OD1	ASP A	180	12.834	-0.224	16.593	1.00127.86	A
MOTA	1404	OD2	ASP A	180	11.256	-1.757	16.465	1.00127.72	A
MOTA	1405	C	ASP A		13.955	-4.772	15.203	1.00127.36	A
ATOM	1406	0	ASP A		14.943	-4.458	14.562	1.00125.75	A
ATOM	1407	N	ALA A		13.708	-5.982	15.682	1.00126.10	A
MOTA	1408	CA	ALA A		14.524	-7.179	15.613	1.00125.36	A
ATOM	1409	CB	ALA A		13.688	-8.331			
ATOM		G	ALA A				16.059	1.00123.72	A
	1410				15.211	-7.562	14.313	1.00125.78	A
ATOM	1411	0	ALA A		15.593	-6.731	13.486	1.00124.90	A
MOTA	1412	N	GLY A		15.415	-8.874	14.232	1.00126.89	A
MOTA	1413	CA	GLY A		16.050	-9.561	13.124	1.00128.12	A
ATOM	1414	C	GLY A			-10.982	13.618	1.00128.80	A
MOTA	1415	0	GLY A			-11.785	13.650	1.00129.69	Α
MOTA	1416	N	SER A			-11.264	14.031	1.00127.74	A
ATOM	1417	CA	SER A			-12.555	14.548	1.00125.79	_ A
ATOM	1418	CB	SER A			-13.710	13.847	1.00126.51	A
MOTA	1419	OG	SER A			-14.862	14.674	1.00126.57	A
MOTA	1420	C	SER A			-12.563	14.192	1.00123.68	A
ATOM	1421	0	SER A			-13.436	14.600	1.00123.14	Α
ATOM	1422	N	asn a	184	19.731	-11.559	13.405	1.00121.45	A
ATOM	1423	CA	asn a	184	21.103	-11.355	12.972	1.00118.98	Α
ATOM	1424	CB	asn a		21.150	-10.362	11.796	1.00119.48	A
ATOM	1425	CG	asn a	184		-10.048	11.346	1.00120.66	A
ATOM	1426	OD1	ASN A	184	23.311	-10.942	10.927	1.00121.24	A
ATOM	1427	ND2	ASN A	184	22.959	-8.773	11.435	1.00119.84	A
ATOM	1428	С	ASN A	184	21.818	-10.771	14.178	1.00115.89	A
MOTA	1429	0	ASN A	184	22.584	-9.807	14.071	1.00115.71	A
MOTA	1430	N	ILE A	185	21.531	-11.348	15.338	1.00111.89	A
MOTA	1431	CA	ILE A	185	22.142	-10.889	16.571	1.00107.91	A
MOTA	1432	CB	ILE A	185	21.827	-11.843	17.736	1.00106.06	A
MOTA	1433	CG2	ILE A	185	22.492	-11.332	19.010	1.00107.39	Α
ATOM	1434	CG1	ILE A	185	20.311	-11.935	17.940	1.00100.90	A
MOTA	1435	CD1	ILE A	185	19.900	-12.804	19.106	1.00 97.34	A
MOTA	1436	C	ILE A	185	23.656	-10.778	16.393	1.00105.30	A
ATOM	1437	0	ILE A	185	24.318	-11.727	15.970	1.00105.17	Α .
MOTA	1438	N	THR A	186	24.189	-9.603	16.707	1.00100.69	A
ATOM	1439	CA	THR A	186	25.612	~9.335	16.563	1.00 93.77	Α
ATOM	1440	CB	THR A	186	25.827	-8.411	15.382	1.00 92.19	A
ATOM	1441	OG1	THR A	186	24.918	-7.307	15.473	1.00 90.68	A
ATOM	1442	CG2	THR A	186	25.555	-9.146	14.097	1.00 92.78	A
ATOM	1443	C	THR A	186	26.212	-8.711	17.818	1.00 89.49	A
MOTA	1444	0	THR A	186	25.590	-7.863	18.462	1.00 88.41	A
ATOM	1445	И	TYR A	187	27.433	-9.116	18.154	1.00 84.65	A
ATOM	1446	CA	TYR A		28.067	-8.604	19.361	1.00 77.64	A
ATOM	1447	CB	TYR A	187	27.500	-9.339	20.560	1.00 71.90	A
MOTA	1448	CG	TYR A			-10.778	20.586	1.00 66.23	A
ATOM	1449		TYR A			-11.133	21.061	1.00 65.84	A
MOTA	1450		TYR A			-12.451	21.061	1.00 64.03	A
MOTA	1451		TYR A			-11.782	20.108	1.00 66.58	A
MOTA	1452		TYR A			-13.106	20.101	1.00 67.83	A
ATOM	1453	CZ	TYR A			-13.432	20.581	1.00 65.88	A
ATOM	1454	ОН	TYR A			-14.741	20.582	1.00 71.57	A
MOTA	1455	C	TYR A		29.572	-8.779	19.395	1.00 74.75	A
ATOM	1456	ŏ	TYR A		30.123	-9.677	18.768	1.00 76.90	A
MOTA	1457	N	ARG A		30.222	-7.920	20.163	1.00 72.05	A
MOTA	1458	CA	ARG A		31.664	-7.984	20.369	1.00 68.17	A
ATOM	1459	CB	ARG A		32.335	-6.736	19.794	1.00 68.30	A
								- · · 	

MOTA	1460	CG	ARG A	188	31.964	-6.447	18.349	1.00 72.52	A
MOTA	1461	CD	ARG A	188	32.486	-5.094	17.891	1.00 72.57	Α
MOTA	1462	NE	ARG A	188	33.938	-5.063	17.772	1.00 79.20	A
MOTA	1463	CZ	ARG A	188	34.626	-5.739	16.857	1.00 83.58	A
ATOM	1464	NHl	ARG A		33.991	-6.500	15.978	1.00 84.25	A
MOTA	1465		ARG A		35.950	-5.654	16.819	1.00 85.58	A
MOTA	1466	C	ARG A		31.759	-7.988	21.898	1.00 64.34	A
MOTA	1467	0	ARG A		30.749	-7.753	22.571	1.00 67.40	A
ATOM	1468	N ·	THR A		32.921	-8.285	22.468	1.00 55.07	A
MOTA	1469	CA	THR A		33.013	-8.235	23.925	1.00 49.47	A
MOTA	1470	CB	THR A		33.019	-9.605	24.575	1.00 41.74	A
ATOM	1471		THR A			-10.186	24.436	1.00 38.57	A
ATOM	1472	CG2	THR A			-10.483	23.959	1.00 40.69	A
ATOM	1473	C	THR A		34.270	-7.512	24.369	1.00 50.81	A
ATOM	1474	ŏ	THR A		35.010	-6.968	23.545	1.00 53.06	A
MOTA	1475	N	ILE A		34.510	-7.493	25.675	1.00 47.66	Ā
ATOM	1476	CA	ILE A		35.678	-6.810	26.188	1.00 43.07	Ā
ATOM	1477	CB	ILE A		35.241	-5.625	27.060	1.00 40.04	A
ATOM	1478	CG2	ILE A		36.442	-4.768	27.443	1.00 37.19	A
ATOM	1479	CG1	ILE A		34.250	-4.776	26.249	1.00 37.15	A
ATOM	1480	CD1	ILE A		33.859	-3.460	26.863	1.00 30.47	A
ATOM	1481	C	ILE A		36.558	-7.796	26.935	1.00 43.76	A
ATOM	1482	ŏ	ILE A		36.153	-8.377	27.942	1.00 46.04	Ā
ATOM	1483	N	ASN A		37.763	-8.001	26.412	1.00 40.93	A
ATOM	1484	CA	ASN A		38.701	-8.947	27.001	1.00 39.01	A
ATOM	1485	CB	ASN A		39.641	-9.487	25.937	1.00 41.88	A
ATOM	1486	CG	ASN A		40.487	-8.393	25.310	1.00 43.26	A
ATOM	1487		ASN A		41.093	-7.562	26.002	1.00 42.40	A
ATOM	1488		ASN A		40.533	-8.389	23.996	1.00 42.40	Â
ATOM	1489	C	ASN A		39.550	-8.364	28.110	1.00 36.32	Ā
ATOM	1490	ō	ASN A		39.580	-7.149	28.332	1.00 36.32	A
ATOM	1491	Ŋ	ASP A			-9.269	28.762	1.00 28.92	A
ATOM	1492	CA	ASP A		41.154	-8.971	29.867	1.00 20.32	A
ATOM	1493	CB	ASP A			-10.152	30.114	1.00 30.28	A
ATOM	1494	CG	ASP A			-11.413	30.558	1.00 37.35	Ä
ATOM	1495		ASP A			-12.372	30.957	1.00 40.37	Ā
ATOM	1496		ASP A			-11.454	30.512	1.00 40.36	Ä
ATOM	1497	C	ASP A		42.003	-7.733	29.674	1.00 32.17	A
ATOM	1498	ŏ	ASP A		42.551	-7.200	30.638	1.00 33.76	A
ATOM	1499	N	TYR A		42.127	-7.262	28.441	1.00 34.99	A
ATOM	1500	CA	TYR A		42.965	-6.096	28.196	1.00 36.95	Ä
ATOM	1501	CB	TYR A		43.944	-6.387	27.060	1.00 38.04	A
ATOM	1502	CG	TYR A		44.606	-7.716	27.256	1.00 38.50	A
ATOM	1503	CD1			44.205	-8.827	26.524	1.00 38.64	A
ATOM	1504	CE1				-10.082	26.774	1.00 44.97	A
ATOM	1505	CD2	TYR A		45.576	-7.889	28.246	1.00 43.23	Ä
ATOM	1506	CE2	TYR A		46.130	-9.134	28.504	1.00 43.94	A
ATOM	1507	CZ	TYR A			-10.229	27.766	1.00 46.01	A
MOTA	1508	OH	TYR A			-11.466	28.010	1.00 46.49	A
ATOM	1509	C	TYR A		42.126	-4.900	27.881	1.00 37.64	Â
ATOM	1510	Ö	TYR A		42.625	-3.876	27.408	1.00 37.04	A
ATOM	1511	N	GLY A		40.839	-5.042	28.163	1.00 39.29	A
ATOM	1512	CA	GLY A		39.915	-3.956	27.929	1.00 39.29	
ATOM	1513	C	GLY A		39.877	-3.936	26.459	1.00 44.48	A
MOTA	1514	õ	GLY A		39.659	-2.541	26.439	1.00 45.55	A
ATOM	1515	И	ALA A			-2.541 -4.737	25.687	1.00 59.09	A
ATOM	1516	CA	ALA A		40.105 40.112	-4.737 -4.664	24.234	1.00 51.50	A
ATOM	1517	CB	ALA A			-4.80 4 -5.308	24.234		A
TON	131/	CD	чти А	1 22	41.388	-5.300	43.03/	1.00 55.95	A

MOTA MOTA MOTA MOTA MOTA	1518 1519 1520 1521	0 N	ALA ALA LEU	Α	195		38.875	-5.363 -6.372	23.663	1.00 52.17 1.00 44.64	A A
MOTA MOTA	1520 1521	N									A
MOTA	1521		LEU	70							
				-	196		38.336	-4.800	22.581	1.00 57.21	A
MOTA	1 - 2 2	CA	$_{ m LEU}$	Α	196		37.156	-5.343	21.914	1.00 59.75	A
	1522	CB	LEU	Α	196		36.579	-4.325	20.925	1.00 61.85	A
MOTA	1523	CG	LEU	A	196		35.802	-3.124	21.471	1.00 67.63	A
MOTA	1524	CD1	LEU	Α	196		35.470	-2.154	20.342	1.00 69.19	A
ATOM	1525		LEU				34.529	-3.609	22.146	1.00 68.00	A
ATOM	1526	C	LEU				37.511	-6.603	21.152	1.00 60.64	A
ATOM	1527	ō	LEU				38.426	-6.606	20.336	1.00 64.49	A
ATOM	1528	N	THR				36.797	-7.684	21.417	1.00 62.05	A
ATOM	1529	CA	THR				37.066	-8.910	20.695	1.00 63.87	A
ATOM	1530	CB	THR					-10.133	21.391	1.00 61.93	
MOTA	1531	OG1						-10.042	21.331	1.00 60.47	A
MOTA	1532	CG2						-10.042	22.833		A
ATOM	1532	C	THR				36.437	-8.709		1.00 59.69	A
ATOM		Ö							19.321	1.00 67.77	A
	1534		THR				35.717	-7.730	19.097	1.00 64.73	A
ATOM	1535	N	PRO				36.709	-9.620	18.377	1.00 71.03	A
ATOM	1536	CD	PRO					-10.802	18.434	1.00 71.83	A
ATOM	1537	CA	PRO				36.130	-9.467	17.044	1.00 73.03	A
MOTA	1538	CB	PRO					-10.440	16.209	1.00 69.75	A
ATOM	1539	CG	PRO					-11.548	17.180	1.00 70.02	A
ATOM	1540	C	PRO				34.633	-9.778	17.023	1.00 75.14	A
ATOM	1541	0	PRO	Α	198		34.160	-10.672	17.733	1.00 76.71	A
ATOM	.1542	N	LYS	Α	199		33.904	-9.022	16.205	1.00 75.43	A
ATOM	1543	CA	LYS	A	199		32.461	-9.174	16.040	1.00 74.90	A
MOTA	1544	CB	LYS	Α	199	•	31.996	-8.239	14.924	1.00 72.98	A
MOTA	1545	CG	LYS	Α	199		30.553	-8.372	14.496	1.00 80.47	A
MOTA	1546	CD	LYS	Α	199		30.224	-7.211	13.545	1.00 88.05	A
MOTA	1547	CE	LYS	Α	199		29.032	-7.494	12.628	1.00 91.80	A
ATOM	1548	NZ	LYS	Α	199		27.748	-7.639	13.354	1.00 91.26	
ATOM	1549	C	LYS	Α	199			-10.618	15.721	1.00 74.91	A
MOTA	1550	o			199			-11.243	14.847	1.00 75.65	A
ATOM	1551	N	MET					-11.156	16.444	1.00 76.24	A
ATOM	1552	CA	MET					-12.524	16.203	1.00 77.12	A
ATOM	1553	CB	MET					-13.418	17.390	1.00 79.60	A
ATOM	1554	CG	MET					-12.807	18.358	1.00 73.80	A
ATOM	1555	SD	MET					-14.062	19.372	1.00 95.64	
ATOM	1556	CE	MET					-13.534	19.372		A
MOTA	1557	C	MET					-12.514	15.981	1.00 90.12	A
ATOM	1558	Ö	MET							1.00 76.38	A
MOTA	1559	И	THR					-11.532	16.310	1.00 74.07	A
MOTA	1560	CA	THR					-13.606	15.430	1.00 77.03	A
	1561		THR					-13.702	15.148	1.00 78.59	A
MOTA		CB						-14.410	13.799	1.00 77.42	· A
ATOM	1562		THR THR					-13.670	12.749	1.00 77.17	A
ATOM	1563							-14.496	13.516	1.00 74.13	A
ATOM	1564	C	THR					-14.412	16.221	1.00 79.06	A
MOTA	1565	0	THR					-15.482	16.703	1.00 78.93	A
MOTA	1566	N	GLY					-13.803	16.575	1.00 80.08	A
MOTA	1567	CA	GLY					-14.374	17.576	1.00 85.07	A
MOTA	1568	C	GLY					-15.781	17.203	1.00 88.30	A
MOTA	1569	0	GLY					-16.041	16.056	1.00 89.73	A
MOTA	1570	N	VAL					-16.684	18.177	1.00 89.55	A
ATOM	1571	CA	VAL				23.701	-18.083	17.958	1.00 91.19	A
MOTA	1572	CB	VAL				24.965	-18.955	18.037	1.00 90.44	A
MOTA	1573		VAL				24.639	-20.396	17.682	1.00 89.78	A
MOTA	1574	CG2	VAL				26.028	-18.389	17.119	1.00 88.29	A
MOTA	1575	С	VAL	Α	203		22.691	-18 579	18.993	1.00 93.60	A

MOTA	1576	0	VAL	Α	203		23.051	-19.320	19.910	1.00 96.4	46 A
MOTA	1577	N	MET	Α	204		21.432		18.837	1.00 94.	
ATOM	1578	CA	MET				20.359	-18.554	19.763	1.00 95.	
MOTA	1579	CB			204	. •		-18.259	19.139	1.00 97.	
ATOM	1580	CG	MET					-16.781	18.846	1.00100.	
ATOM	1581	SD	MET				19.848	-16.028	17.632	1.00100.	
ATOM	1582	CE			_						
			MET					-16.409	16.081	1.00106.4	
ATOM	1583	C	MET					-20.022	20.175	1.00 95.4	
MOTA	1584	0	MET					-20.902	19.337	1.00 94.	
MOTA	1585	N	GLU					-20.282	21.471	1.00 97.	70 A
MOTA	1586	CA	GLU	А	205		20.343	-21.651	21.968	1.00101.2	28 A
ATOM	1587	CB	GLU	A	205		20.877	-21.711	23.403	1.00104.8	34 A
MOTA	1588	CG	GLU	Α	205		19.906	-21.187	24.466	1.00112.5	54 A
MOTA	1589	CD	GLU	Α	205		19.661	-22.185	25.597	1.00116.3	36 A
MOTA	1590	OE1	GLU	Α	205		18.893	-21.859	26.535	1.00117.1	
ATOM	1591	OE2	GLU	Α	205		20.234	-23.296	25.544	1.00117.6	
ATOM	1592	С	GLU				18.933	-22.211	21.939	1.00102.6	
ATOM	1593	0	GLU					-23.396	21.575	1.00102.5	
ATOM	1594		GLU				18.003	-21.453	22.299	1.00103.8	
ATOM	1595	СВ	PHE		1			-11.695	6.773		
ATOM	1596	CG	PHE		ī			-11.042	7.714	1.00 32.6	
ATOM	1597		PHE		ī					1.00 34.2	
ATOM								-10.867	7.347	1.00 36.1	
	1598		PHE		1			-10.662	8.993	1.00 31.5	
ATOM	1599		PHE		1			-10.333	8.242	1.00 29.9	
ATOM	1600		PHE		1			-10.122	9.898	1.00 30.3	
MOTA	1601	CZ	PHE		1		79.514	-9.962	9.519	1.00 32.6	
ATOM ·	1602	C	PHE		1		80.968	-13.803	6.514	1.00 32.7	70 B
ATOM	1603	0	$_{ m PHE}$	В	1		80.485	-13.669	5.389	1.00 29.6	58 B
ATOM	1604	N	PHE	В	. 1		83.310	-13.795	5.858	1.00 39.6	55 B
MOTA	1605	CA	PHE	В	1		82.342	-13.237	6.842	1.00 35.4	4 B
MOTA	1606	N	ALA	В	2		80.360	-14.460	7.496	1.00 31.7	/1 B
MOTA	1607	CA	ALA	В	2		79.040	-15.055	7.321	1.00 30.8	32 B
MOTA	1608	CB	ALA	В	2		79.189	-16.485	6.894	1.00 21.9	
ATOM	1609	C	ALA	В	2			-14.976	8.631	1.00 30.4	
ATOM	1610	0	ALA		2			-14.856	9.707	1.00 29.1	
ATOM	1611	N	CYS		3			-15.045	8.549	1.00 24.6	
ATOM	1612	CA	CYS		3			-14.973	9.755	1.00 25.8	
ATOM	1613	C	CYS		3			-16.076	9.766	1.00 25.8	_
ATOM	1614	0	CYS		3			-16.636	8.731		
ATOM	1615	CB	CYS		3			-13.618		1.00 27.4	
ATOM	1616	SG	CYS		3			-12.127	9.847	1.00 29.9	_
									9.708	1.00 38.2	
MOTA	1617	N	LYS		4			-16.390	10.942	1.00 28.1	
ATOM	1618	CA	LYS		4			-17.423	11.060	1.00 31.7	_
MOTA	1619	CB	LYS		4			-18.786	11.447	1.00 28.6	_
ATOM	1620	CG	LYS		4			-18.828	12.846	1.00 40.2	_
ATOM	1621	CD	LYS		4			-20.146	13.165	1.00 46.8	
MOTA	1622	CE	LYS		4			-21.313	13.324	1.00 57.6	3 B
MOTA	1623	NZ	LYS		4			-21.671	12.052	1.00 66.2	21 B
MOTA	1624	C	LYS	В	4		72.502	-17.025	12.096	1.00 34.5	54 B
MOTA	1625	0	LYS	В	4		72.742	-16.198	12.972	1.00 33.5	
ATOM	1626	N	THR	В	5		71.348	-17.653	11.982	1.00 36.2	
ATOM	1627	CA	THR		5			-17.395	12.852	1.00 35.5	
ATOM	1628	СВ	THR		~ 5			-17.255	11.990	1.00 33.2	_
ATOM	1629	OG1	THR		5			-16.064	12.371	1.00 39.6	
ATOM	1630	CG2	THR		5			-18.440	12.114	1.00 33.8	
ATOM	1631	C	THR		5			-18.515	13.873	1.00 21.0	_
ATOM	1632	o	THR		5			-19.685			
ATOM	1633	N							13.544	1.00 39.7	
WI OIL	T022	TA	ALA	D	6		07.741	-18.141	15.124	1.00 37.3	86 B

MOTA	1634	CA	ALA :	в 6		-19.100	16.217	1.00 37.84	В
MOTA	1635	CB	ALA :	В б	69.476	-18.389	17.505	1.00 37.58	В
MOTA	1636	C	ALA :	B 6	68.840	-20.172	15.907	1.00 41.46	В
MOTA	1637	0	ALA :	В 6	68.921	-21.289	16.413	1.00 43.45	В
MOTA	1638	N	ASN :	в 7	67.877	-19.830	15.064	1.00 48.11	В.
ATOM	1639	CA	ASN :	в 7	66.832	-20.774	14.690	1.00 52.20	В
ATOM	1640	CB	ASN :	в 7	65.690	-20.040	14.008	1.00 54.22	В
MOTA	1641	CG	ASN			-20.578	14.405	1.00 55.97	В
ATOM	1642		ASN			-21.579	15.121	1.00 57.99	В
ATOM	1643		ASN			-19.920	13.945	1.00 50.39	В
ATOM	1644	C	ASN			-21.833	13.756	1.00 51.16	В
ATOM	1645	Ö	ASN :			-22.998	13.824	1.00 55.83	В
ATOM	1646	N	GLY :			-21.410	12.884	1.00 50.20	В
MOTA	1647	CA	GLY :			-22.318	11.940	1.00 55.38	
ATOM		CA	GLY :			-22.318	10.708		В
	1648							1.00 59.62	В
ATOM	1649	0	GLY :			-21.908	10.370	1.00 62.92	В
ATOM	1650	N	THR 1			-20.777	10.055	1.00 54.57	В
ATOM	1651	CA	THR			-20.093	8.820	1.00 49.33	В
MOTA	1652	CB	THR 1			-19.233	8.317	1.00 48.69	. В
MOTA	1653		THR I			-20.062	8.173	1.00 56.73	В
MOTA	1654		THR I			-18.617	6.976	1.00 49.41	В
MOTA	1655	С	THR I			-19.265	8.772	1.00 47.43	В
MOTA	1656	0	THR I	в 9	70.772	-18.598	9.733	1.00 49.84	В
MOTA	1657	N	ALA 1	B 10	71.071	-19.311	7.617	1.00 43.83	₿
MOTA	1658	CA	ALA :	B 10	72.330	-18.606	7.394	1.00 39.16	В
MOTA	1659	CB	ALA 1	B 10	73.463	-19.607	7.265	1.00 31.66	В
MOTA	1660	C	ALA 1	B 10	72.323	-17.741	6.159	1.00 37.14	В
ATOM	1661	0	ALA I	B 10	71.521	-17.942	5.252	1.00 38.98	В
ATOM	1662	N	ILE 1	B 11	73.223	-16.767	6.144	1.00 32.97	· в
MOTA	1663	CA	ILE 1	B 11	73.404	-15.896	5.001	1.00 33.22	В
ATOM	1664	CB	ILE 1	B 11	73.107	-14.448	5.317	1.00 34.97	В
ATOM	1665	CG2	ILE 1	B 11	73.322	-13.616	4.063	1.00 33.99	В
MOTA	1666	CG1	ILE !	B 11	71.671	-14.320	5.838	1.00 36.23	В
ATOM	1667		ILE I			-12.903	6.198	1.00 35.08	В
ATOM	1668	C	ILE I			-16.060	4.767	1.00 33.83	В
ATOM	1669	ō	ILE I			-15.729	5.617	1.00 43.80	В
ATOM	1670	N	PRO I			-16.575	3.609	1.00 30.79	В
ATOM	1671	CD	PRO 1			-16.999	2.492	1.00 34.49	В
ATOM	1672	CA	PRO 1			-16.797	3.290	1.00 31.29	В
ATOM	1673	CB	PRO 1			-17.816	2.164	1.00 33.05	В
ATOM	1674	CG	PRO I			-17.288	1.380	1.00 29.85	В
ATOM	1675	C	PRO			-15.596	2.889	1.00 32.87	В
ATOM	1676	ŏ	PRO			-14.472	2.791	1.00 32.44	. в
ATOM	1677	N	ILE I			-15.881	2.657	1.00 32.91	. В
ATOM	1678	CA	ILE :			-14.910	2.205	1.00 32.69	
		CB	ILE			-14.510			В
ATOM	1679						1.778	1.00 32.47	В
ATOM	1680		ILE I			-14.688	0.989	1.00 30.76	В
ATOM	1681		ILE I			-16.194	3.018	1.00 30.76	В
ATOM	1682		ILE I			-16.954	2.715	1.00 22.14	В
ATOM	1683	C	ILE !	_		-14.195	0.989	1.00 31.24	В.
ATOM	1684	0	ILE I			-14.851	0.082	1.00 35.40	В
ATOM	1685	N	GLY 1			-12.868	0.970	1.00 27.66	В
MOTA	1686	CA	GLY :			-12.129	-0.159	1.00 29.28	В
MOTA	1687	C	GLY :			-11.498	0.150	1.00 33.58	В
ATOM	1688	0	GLY 1			-10.704	-0.631	1.00 32.37	В
MOTA	1689	N	GLY 1			-11.867	1.289	1.00 34.26	В
MOTA	1690	CA	GLY :			-11.294	1.676	1.00 32.52	В
MOTA	1691	C	GLY I	B 15	74.313	-12.041	1.202	1.00 33.57	В

ATOM	1692	0	GLY	в :	15	74.405	-13.053	0.513	1.00	35.21	В
MOTA	1693	N	GLY	в :	16	73.150	-11.514	1.577	1.00	30.98	· В
ATOM	1694	CA	GLY	в :	16	71.887	-12.126	1.224	1.00	23.66	В
ATOM	1695	С	GLY	в :	16	70.874	-11.761	2.281	1.00	22.40	В
MOTA	1696	0	GLY	в :	16	71.011	-10.742	2.944	1.00	26.18	В
ATOM	1697	N	SER	в :	17	69.866	-12.584	2.492	1.00	19.46	В
ATOM	1698	CA	SER	-	17		-12.199	3.478		19.03	В
ATOM	1699	CB	SER		17		-11.375	2.796		25.66	В
ATOM	1700	OG	SER		17		-12.199	2.016		32.12	В
ATOM	1701	C	SER		17		-13.369	4.197		16.25	В
ATOM		Ö	SER		17		-14.476	3.679			
	1702	_								18.07	В
ATOM	1703	N	ALA		18		-13.124	5.396		15.13	В
ATOM	1704	CA	ALA		18		-14.188	6.160		13.99	В
MOTA	1705	CB	ALA		18		-14.934	6.969		11.08	В
MOTA	1706	С	ALA		18		-13.676	7.073		19.72	В
ATOM	1707	0	ALA		18		-12.498	7.438		26.53	В
MOTA	1708	N	ASN		19		-14.582	7.439		20.77	В
MOTA	1709	CA	ASN		19		-14.275	8.344		19.46	В
MOTA	1710	CB	asn		19	62.847	-15.181	8.073	1.00	15.18	В
MOTA	1711	CG	ASN		19	62.037	-14.739	6.870	.1.00	18.55	В
MOTA	1712	OD1	asn	в :	19	62.378	-13.761	6.202	1.00	11.36	В
ATOM	1713	ND2	asn	в :	19	60.955	-15.464	6.584	1.00	8.90	В
ATOM	1714	С	ASN	B 3	19	64.495	-14.532	9.764	1.00	22.89	В
ATOM	1715	0	ASN	в :	19	65.205	-15.491	10.038	1.00	25.04	В
MOTA	1716	N	VAL	B 2	20	64.067	-13.682	10.681	1.00	26.63	В
ATOM	1717	CA	VAL	В 2	20	64.379	-13.907	12.078	1.00	28.04	В
ATOM	1718	CB	VAL	В 2	20	65.314	-12.842	12.589	1.00	27.80	В
ATOM	1719		VAL		20		-13.190	14.000		29.15	В
ATOM	1720		VAL		20		-12.759	11.663	1.00		В
ATOM	1721	C	VAL		20		-13.885	12.840	1.00		В
MOTA	1722	ō	VAL	_	20		-12.845	12.935	1.00		В
ATOM	1723	N	TYR		21		-15.041	13.355	1.00		В
ATOM	1724	CA	TYR		21		-15.181	14.091	1.00		В
ATOM	1725	CB	TYR		21		-16.553	13.802	1.00		В
ATOM	1726	CG	TYR		21.		-16.848	12.333	1.00		В
ATOM	1727		TYR		21		-17.673	11.741	1.00		В
ATOM	1728	CE1	TYR		21		-17.918	10.364	1.00		В
ATOM	1729	CD2	TYR		21		-16.266	11.513	1.00		
		CE2	TYR		21						В
ATOM	1730						-16.505	10.141	1.00		В
MOTA	1731	CZ	TYR		21		-17.335	9.575		31.58	В
MOTA	1732	OH	TYR		21		-17.607	8.234		35.73	В
ATOM	1733	C	TYR		21		-14.973	15.615	1.00		В
ATOM	1734	0	TYŖ		21		-15.747	16.321		33.69	В
ATOM	1735	N	VAL		22		-13.952	16.122		29.81	, B
ATOM	1736	CA	VAL		22		-13.611	17.550		28.88	B
ATOM	1737	CB	VAL		22		-12.189	17.758	1.00		В
ATOM	1738		VAL		22 .		-12.019	17.142	1.00		В
ATOM	1739		VAL		22		-11.227	17.160		18.87	В
MOTA	1740	С	VAL		22		-13.677	18.362	1.00		В
ATOM	1741	0	VAL		22		-13.181	17.931		29.65	В
MOTA	1742	N	ASN		23		-14.266	19.554	1.00		В
ATOM	1743	CA	ASN		23		-14.333	20.478		32.32	В
MOTA	1744	CB	asn		23	58.638	-15.560	21.343	1.00	33.67	В
ATOM ·	1745	CG	ASN	в :	23	59.048	-16.761	20.566	1.00	34.47	В
MOTA	1746		ASN		23	58.219	-17.500	20.030	1.00	31.16	В
ATOM	1747	ND2	ASN	B 2	23	60.349	-16.960	20.474	1.00	42.29	В
ATOM	1748	C	ASN		23	58.675	-13.088	21.353	1.00	32.53	В
MOTA	1749	0	ASN	в :	23	59.720	-12.881	21.971	1.00	27.61	В

MOTA	1750	N	LEU	В	24	57.639	-12.258	21.392	1.00 33.86	В
ATOM	1751	CA	LEU	В	24	57.683	-11.015	22.166	1.00 34.98	В
ATOM	1752	СВ	LEU		24	57.233	-9.857	21.273	1.00 33.61	
										В
MOTA	1753	CG	LEU		24	57.914	-9.705	19.909	1.00 25.28	В
ATOM	1754	CD1	LEU	В	24	56.962	-9.013	18.959	1.00 19.99	В
ATOM	1755	CD2	LEU	В	24	59.196	-8.912	20.028	1.00 29.84	В
ATOM	1756	C	LEU	R	24	56.796	-11.047	23.416	1.00 34.24	В
ATOM	1757	ō	LEU		24		-11.849			
								23.500	1.00 38.70	В
ATOM	1758	N	ALA		25		-10.181	24.386	1.00 29.44	В
MOTA	1759	CA	ALA	В	25	56.266	-10.087	25.601	1.00 26.87	В
MOTA	1760	CB	ALA	В	25	56.657	-8.867	26.375	1.00 21.78	В
ATOM	1761	C	ALA	В	25	54.814	-9.958	25.138	1.00 29.09	В
ATOM	1762	ŏ	ALA		25	54.484	-9.078	24.361	1.00 36.37	В
MOTA							-10.814			
	1763	N	PRO		26			25,619	1.00 27.06	В
MOTA	1764	CD	PRO		26		-11.844	26.637	1.00 28.83	В
MOTA	1765	CA	PRO	В	26	52.513	-10.761	25.206	1.00 31.81	В
MOTA	1766	CB	PRO	В	26	51.888	-11.976	25.921	1.00 32.26	В
ATOM	1767	CG	PRO	В	26	53.043	-12.835	26.271	1.00 36.18	В
ATOM	1768	C	PRO			51.726	-9.473	25.512	1.00 32.59	- B
ATOM	1769	ō	PRO		26	50.748	-9.150	24.825		
									1.00 27.68	В
ATOM	1770	N	VAL		27	52.154	-8.766	26.553	1.00 33.23	В
ATOM	1771	CA	VAL	В	27	51.508	-7.548	27.009	1.00 30.33	В
ATOM	1772	CB	VAL	В	2 7	50.729	-7.814	28.299	1.00 32.83	В
ATOM	1773	CG1	VAL	В	27	50.191	-6.519	28.863	1.00 34.49	В
ATOM	1774		VAL		27	49.615	-8.812	28.038	1.00 34.69	В
ATOM	1775	C	VAL		27	52.517	-6.468	27.327	1.00 31.47	
										В
MOTA	1776	0	VAL		27	53.525	-6.720	27.968	1.00 36.58	В
MOTA	1777	N	VAL		28	52.228	-5.250	26.907	1.00 33.06	В
ATOM	1778	CA	VAL	В	28	53.110	-4.131	27.175	1.00 34.52	В
ATOM	1779	CB	VAL	В	28	54.048	-3.875	25.979	1.00 33.98	В
ATOM	1780	CG1	VAL	B	28	55.047	-2.765	26.297	1.00 34.51	В
ATOM	1781		VAL		28	54.775	-5.146	25.634	1.00 35.52	B
ATOM		· C								
			VAL		28	52.183	-2.944	27.391	1.00 39.51	В
ATOM	1783	0	VAL		28	51.196	-2.778	26.663	1.00 42.77	В
MOTA	1784	N	ASN		29	52.488	-2.123	28.392	1.00 39.90	В
MOTA	1785	CA	ASN	В	29	51.639	-0.977	28.695	1.00 38.73	В
ATOM	1786	CB	ASN	В	29	51.529	-0.748	30.199	1.00 31.74	В
ATOM	1787	CG	ASN		29	51.026	-1.952	30.926	1.00 35.82	В
ATOM	1788	_	ASN		29	49.958	-2.465	30.611	1.00 38.41	
										В
MOTA	1789		ASN		29	51.794	-2.425	31.910	1.00 41.70	В
ATOM	1790	C	ASN		29	52.186	0.275	28.088	1.00 38.86	В
ATOM	1791	0	ASN	В	29	53.385	0.374	27.815	1.00 33.54	В
MOTA	1792	N	VAL	В	30	51.292	1.237	27.891	1.00 37.78	В
ATOM	1793	CA	VAL	В	30	51.695	2.513	27.354	1.00 38.82	В
ATOM	1794	СВ	VAL		30	50.525	3.522	27.378	1.00 37.94	B
ATOM	1795		VAL		30					
						50.989	4.887	26.880	1.00 30.95	В
ATOM	1796		VAL		30	49.387	3.013	26.507	1.00 35.51	В
MOTA	1797	C	VAL	В	30	52.773	2.949	28.334	1.00 41.89	В
ATOM	1798	0	VAL	В	30	52.678	2.651	29.526	1.00 37.14	В
MOTA	1799	N	GLY	В	31	53.813	3.610	27.832	1.00 45.72	В
ATOM	1800	CA	GLY		31	54.879	4.066	28.706	1.00 48.04	В
ATOM	1801	C	GLY		31		3.080	28.893	1.00 50.10	
						56.019				В
ATOM	1802	0	GLY		31	57.159	3.493	29.086	1.00 52.11	В
ATOM	1803	N	GIM		32	55.726	1.785	28.841	1.00 49.45	` В
MOTA	1804	CA	GLN	В	32	56.755	0.765	29.009	1.00 50.86	В
ATOM	1805	СВ	GLN		32	56.115	-0.528	29.500	1.00 51.28	В
ATOM	1806	CG	GLN		32	56.016	-0.625	31.006	1.00 63.66	В
ATOM	1807	CD	GLN		32	55.049	-1.711	31.456	1.00 69.42	В
		22	J1111	_	54	JJ.049,		J. 1. 4.50	1.00 07.42	ם

MOTA	1808	OE1	GLN B	32	55.004	-2.806	30.875	1.00 67.50	В
MOTA	1809	NE2	GLN B	32	54.271	-1.417	32.506	1.00 69.01	В
MOTA	1810	C	GLN B	32	57.578	0.477	27.744	1.00 52.35	В
ATOM	1811	0	GLN B	32	57.339	1.044	26.673	1:00 52.23	В
ATOM	1812	N	ASN B	33	58.560	-0.408	27.892	1.00 49.97	В
ATOM	1813	CA	ASN B	33	59.431	-0.804	26.791	1.00 45.57	В
ATOM	1814	CB	ASN B	33	60.894		27.186	1.00 38.58	В
ATOM	1815	CG	ASN B	33	61.487	0.663	26.722	1.00 42.92	В
ATOM	1816		ASN B	33	62.591	1.031	27.126	1.00 40.10	В
ATOM	1817		ASN B	33	60.774	1.367	25.854	1.00 40.86	В
ATOM	1818	C	ASN B	33	59.230	-2.245	26.341	1.00 46.44	В
ATOM	1819	Ö	ASN B	33	59.157	-3.180	27.144	1.00 46.44	
ATOM	1820	N	LEU B	34	59.105	-2.418	25.039	1.00 49.81	В
ATOM	1821	CA	LEU B	34	59.007	-3.747	24.470	1.00 49.23	В
ATOM	1822	CB	LEU B	34	58.045	-3.74	-	1.00 48.80	В
ATOM	1823	CG	LEU B	34	58.103	-5.057	23.293		В
ATOM	1824		LEU B	34	57.402			1.00 45.79	B
ATOM	1825		LEU B	34	57.451	-6.200	23.193	1.00 41.87	В
ATOM	1826	CDZ	LEU B			-4.778	21.133	1.00 49.38	В
			LEU B	34	60.445	-3.902	23.976	1.00 48.23	В
ATOM	1827	0		34	60.992	-3.012	23.298	1.00 41.48	В
ATOM	1828	N	VAL B	35	61.077	-5.005	24.334	1.00 47.30	В
MOTA	1829	CA	VAL B	35	62.450	-5.185	23.916	1.00 47.76	В
ATOM	1830	CB	VAL B	35	63.375	-5.332	25.139	1.00 51.29	В
ATOM	1831		VAL B	35	64.819	-5.444	24.689	1.00 50.08	В
ATOM	1832		VAL B	35	63.200	-4.128	26.056	1.00 46.83	В
ATOM	1833	C	VAL B	35	62.644	-6.368	22.998	1.00 42.61	В
ATOM	1834	0	VAL B	35	62.279	-7.497	23.333	1.00 42.72	В
ATOM	1835	N	VAL B	36	63.201		21.824	1.00 38.28	В
MOTA	1836	CA	AMT B	36	63.474	-7.164	20.867	1.00 37.43	В
MOTA	1837	CB	VAL B	36	62.937	-6.861	19.477	1.00 35.42	В
MOTA	1838		VAL B	36	62.693	-8.158	18.759	1.00 38.88	В
ATOM	1839		VAL B	36	61.674	-6.048	19.570	1.00 32.55	В
MOTA	1840	C	VAL B	36	64.974	-7.229	20.790	1.00 36.36	В
MOTA	1841	0	VAL B	36	65.614	-6.363	20.186	1.00 36.91	В
MOTA	1842	N	ASP B	37	65.544	-8.241	21.429	1.00 37.46	В
MOTA	1843	CA	ASP B	37	66.993	-8.380	21.442	1.00 40.31	В
MOTA	1844	CB	ASP B	37	67.456	-8.800	22.835	1.00 44.25	В
MOTA	1845	CG	ASP B	37	68.953	-8.744	22.984	1.00 52.42	В
ATOM	1846	OD1	ASP B	37	69.557	-7.715	22.582	1.00 55.50	В
ATOM	1847	OD2	ASP B	37	69.523	-9.726	23.506	1.00 58.75	В
ATOM	1848	C	ASP B	37	67.473	-9.382	20.404	1.00 35.79	В
ATOM	1849	0	ASP B	37	67.346	-10.593	20.587	1.00 35.22	В
ATOM	1850	N	LEU B	38	68.039	-8.875	19.318	1.00 33.36	В
MOTA	1851	CA	LEU B	38	68.506	-9.757	18.255	1.00 38.32	В
MOTA	1852	CB	LEU B	38	68.451	-9.022	16.917	1.00 34.94	В
MOTA	1853	CG	LEU B	38	66.983	-8.711	16.654	1.00 28.92	В
MOTA	1854	CD1	LEU B	38	66.877	-7.753	15.538	1.00 45.30	В
MOTA	1855		LEU B	38	. 66.230	-9.975	16.340	1.00 28.07	В
ATOM	1856	C	LEU B	38		-10.374	18.487	1.00 36.75	В.
ATOM	1857	ō	LEU B	38		-11.406	17.886	1.00 32.86	В
ATOM	1858	N	SER B	39	70.645	-9.748	19.378	1.00 38.02	В
ATOM	1859	CA	SER B	39		-10.218	19.760	1.00 36.96	В
ATOM	1860	CB	SER B	39	72.558	-9.367	20.880	1.00 42.14	В
MOTA	1861	OG	SER B	39	72.044	-9.821	22.122	1.00 42.14	В
MOTA	1862	C	SER B	39		-11.615	20.305	1.00 40.54	
MOTA	1863	0	SER B	39		-12.321	20.531	1.00 30.79	В
ATOM	1864	И	THR B	40		-12.321	20.531	1.00 33.51	B
ATOM		CA	THR B	40		-13.322	21.042	1.00 29.18	В
ATOM	1865	CA	TUK B	40	10.321	-13.322	41.042	1.00 28.75	В

MOTA	1866	CB	THR E	3 40	69.186	-13.277	22.071	1.00 29.43	В
MOTA	1867	OG1	THR I	3 40	69.692	-13.707	23.334	1.00 32.38	В
MOTA	1868	CG2	THR E	3 40	68.022	-14.163	21.664	1.00 22.59	В
ATOM	1869	С	THR I	3 40		-14.233	19.890	1.00 29.83	В
ATOM	1870	0	THR E			-15.457	20.046	1.00 29.41	В
ATOM	1871	N	GLN I			-13.646	18.721	1.00 31.06	В
ATOM	1872	CA	GLN E		•	-14.460	17.582	1.00 36.78	В
ATOM	1873	CB	GLN E			-14.194	17.264	1.00 40.36	В
ATOM	1874	CG	GLN E			-14.642	18.369	1.00 43.67	В
ATOM	1875	CD	GLN E			-15.289	17.820	1.00 43.67	В
ATOM	1876	OE1	GLN E			-14.617	17.328	1.00 56.24	
MOTA	1877	NE2				-16.615	17.863	1.00 56.24	В
ATOM	1878	C	GLN E			-14.351		1.00 36.15	В
MOTA	1879	0	GLN E			-15.132	16.301		В
ATOM		И	ILE E				15.372 16.250	1.00 31.94	В
MOTA	1880					-13.402		1.00 33.39	В
	1881	CA	ILE E			-13.220	15.052	1.00 32.83	В
MOTA	1882	CB CG2	ILE E			-11.927	14.339	1.00 29.07	В
MOTA	1883		-			-11.772	13.064	1.00 37.11	В.
MOTA			ILE E			-11.956	14.008	1.00 29.91	В
ATOM	1885		ILE E			-10.650	13.455	1.00 32.72	В
MOTA	1886	C .	ILE E			-13.207	15.363	1.00 35.46	В
ATOM	1887	0	ILE E			-12.349	16.108	1.00 34.54	В
ATOM	1888	N	PHE E			-14.168	14.773	1.00 39.21	В
MOTA	1889	CA	PHE E			-14.328	14.971	1.00 38.93	В
MOTA	1890	CB	PHE F			-15.645	15.676	1.00 35.81	В
MOTA	1891	CG	PHE E		_	-15.776	16.979	1.00 37.08	В
MOTA	1892		PHE E			-16.211	17.038	1.00 36.05	В
MOTA	1893		PHE F			-15.399	18.158	1.00 39.14	В
MOTA	1894					-16.266	18.256	1.00 37.91	В
MOTA	1895		PHE E	_		-15.448	19.382	1.00 40.87	В
MOTA	1896	CZ	PHE E	3 43	73.752	-15.882	19.435	1.00 40.29	В
MOTA	1897	C	PHE E	3 43	76.342	-14.288	13.706	1.00 38.93	В
ATOM	1898	0	PHE E	3 43	75.952	-14.807	12.667	1.00 42.09	В
MOTA	1899	N	CYS E	3 44	77.510	-13.681	13.806	1.00 39.28	В
MOTA	1900	CA	CYS E	3 44	78.413	-13.609	12.672	1.00 41.35	В
MOTA	1901	C	CYS E	3 44	79.836	-14.004	13.111	1.00 42.43	В
MOTA	1902	0	CYS E	3 44	80.124	-14.157	14.304	1.00 41.46	В
MOTA	1903	CB	CYS E	3 44		-12.201	12.097	1.00 42.60	В
ATOM	1904	SG	CYS E	3 44	76.786	-11.538	11.633	1.00 48.45	В
MOTA	1905	N	HIS E	3 45	80.719	-14.192	12.141	1.00 41.61	В
MOTA	1906	CA	HIS E	3 45	82.091	-14.563	12.440	1.00 38.21	В
MOTA	1907	CB	HIS E	3 45	82.222	-16.073	12.632	1.00 35.18	В
MOTA	1908	CG	HIS E	3 45	82.034	-16.856	11.372	1.00 40.84	В
MOTA	1909	CD2	HIS F	3 45	82.782	-16.926	10.244	1.00 42.07	В
ATOM	1910	ND1	HIS E	3 45	80.931	-17.648	11.146	1.00 43.80	В
ATOM	1911	CE1	HIS E	3 45	81.003	-18.168	9.934	1.00 43.34.	В
MOTA	1912		HIS E		82.117	-17.745	9.365 [.]	1.00 40.53	В
ATOM	1913	C	HIS E			-14.139	11.272	1.00 37.82	В
MOTA	1914	Ó	HIS E			-13.968	10.164	1.00 39.67	В
ATOM	1915	N	ASN E			-13.967	11.539	1.00 40.18	В
ATOM	1916	CA	ASN E			-13.580	10.544	1.00 38.78	В
MOTA	1917	СВ	ASN E			-12.864	11.260	1.00 38.86	В
ATOM	1918	CG	ASN E			-12.123	10.314	1.00 38.90	В
ATOM	1919		ASN E			-12.626	9.248	1.00 39.63	В
ATOM	1920		ASN E			-10.923	10.706	1.00 26.83	. B
ATOM	1921	C	ASN E		-	-14.915	9.969	1.00 20.03	В
ATOM	1922	0	ASN I			-15.875	10.715	1.00 39.32	В
ATOM	1923	И	ASP I			-15.007	8.665	1.00 40.20	В
			ك خاصدى	1	00.943	~~· · · · · /	0.003	~ · · · · · · · · · · · · · · · · · · ·	₽

MOTA	1924	CA	ASP		47	86.397	-16.288	8.109	1.00 45.	88 B
MOTA	1925	CB	ASP		47	85.789	-16.522	6.712	1.00 43.	41 B
MOTA	1926	CG	ASP		47	84.333	-17.003	6:768	1.00 46.	32 B
ATOM	1927		ASP		47	84.062	-18.030	7.430	1.00 48.	27 B
MOTA	1928		ASP	В	47	83.452	-16.363	6.143	1.00 46.	10 B
MOTA	1929	C	ASP		47	87.927	-16.396	8.050	1.00 46.	45 B
MOTA	1930	0	ASP	В	47	88.492	-17.491	8.051	1.00 43.	03 B
MOTA	1931	N	TYR	В	48	88.595	-15.252	8.001	1.00 47.	00 B
MOTA	1932	CA	TYR	В	48	90.044	-15.233	7.954	1.00 48.	77 B
MOTA	1933	CB	TYR	В	48	90.527	-14.981	6.528	1.00 49.	76 B
MOTA	1934	CG	TYR	В	48	89.944	-15.952	5.520	1.00 56.	
MOTA	1935	CD1	TYR	В	48	88.788	-15.629	4.804	1.00 60.	39 B
MOTA	1936	CE1	TYR	В	48	88.223	-16.525	3.898	1.00 62.	58 B
MOTA	1937	CD2	TYR	В	48	90.527	-17.204	5.301	1.00 58.	
ATOM	1938	CE2	TYR		48	89.967	-18.114	4.393	1.00 61.	62 B
MOTA	1939	cz	TYR	В	48	88.813	-17.764	3.701	1.00 61.	55 B
ATOM	1940	OH	TYR	В	48	88.220	-18.658	2.842	1.00 60.3	24 B
MOTA	1941	C	TYR	В	48	90.542	-14.149	8.896	1.00 48.	73 B
ATOM	1942	0	TYR		48		-13.144	8.465	1.00 49.	92 B
MOTA	1943	N	PRO	В	49	90.328	-14.351	10.207	1.00 47.	96 B
MOTA	1944	CD	PRO	В	49	89.711	-15.557	10.787	1.00 49.3	35 B
MOTA	1945	CA	PRO	В	49	90.730	-13.422	11.263	1.00 49.	89 B
MOTA	1946	CB	PRO	В	49	90.365	-14.173	12.545	1.00 48.	55 B
MOTA	1947	CG	PRO	В	49		-15.604	12.140	1.00 48.3	17 B
MOTA	1948	C	PRO	В	49	92.189	-12.973	11.234	1.00 54.3	32 B
MOTA	1949	0	PRO	В	49	92.461	-11.773	11.151	1.00 55.6	57 B
MOTA	1950	N	GLU	В	50	93.116	-13.932	11.283	1.00 55.	77 B
ATOM	1951	CA	GLU	В	50	94.560	-13.647	11.281	1.00 54.3	39 B
MOTA	1952	CB	GLU		50	95.366	-14.937	11.142	1.00 45.	75 B
MOTA	1953	CG	GLU		50	94.999	-16.029	12.112	1.00 54.0	03 B
MOTA	1954	CD	GLU		50		-16.722	11.739	1.00 62.	75 B
MOTA	1955	OE1			50	93.232	-16.533	10.590	1.00 65.6	50 B
MOTA	1956	OE2			50		-17.467	12.587	1.00 62.8	32 B
MOTA	1957	C	GLU		50		-12.660	10.236	1.00 53.7	74 B
ATOM	1958	0	GLU		50		-12.091	10.431	1.00 58.2	
MOTA	1959	N	THR		51		-12.446	9.138	1.00 49.2	•
ATOM	1960	CA	THR		51		-11.538	8.117	1.00 53.2	
ATOM	1961	CB	THR		51		-12.336	6.885	1.00 53.6	
MOTA	1962	OG1	THR		51		-12.620	5.986	1.00 51.3	
MOTA	1963	CG2	THR		51		-13.657	7.345	1.00 55.7	
MOTA	1964	C	THR		51		-10.520	7.666	1.00 57.3	
MOTA	1965	0	THR		51	94.171	-9.543	6.970	1.00 58.2	
ATOM	1966	N	ILE		52		-10.740	8.060	1.00 54.9	
MOTA	1967	CA	ILE		52	91.558	-9.819	7.670	1.00 49.8	
ATOM	1968	CB	ILE		52		-10.447	6.619	1.00 53.3	
ATOM	1969	CG2	ILE		.52		-9.484	6.275	1.00 54.2	
MOTA	1970		ILE		52		-10.797	5.370	1.00 51.5	
MOTA	1971		ILE		52		-11.461	4.269	1.00 46.6	
ATOM	1972	C	ILE		52	90.725	-9.400	8.850	1.00 49.0	
ATOM	1973	0	ILE		52		-10.218	9.700	1.00 47.5	
ATOM	1974	N ·			53.	90.424	-8.107	8.914	1.00 50.0	
ATOM	1975	CA	THR		53	89.591	-7.574	9.982	1.00 51.3	
MOTA	1976	CB	THR		53	90.272	-6.389	10.703	1.00 52.9	
ATOM	1977		THR		53	91.205	-6.892	11.669	1.00 51.3	
ATOM	1978	CG2			53	89.238	-5.524	11.415	1.00 50.4	
ATOM	1979	C	THR		53	88.265	-7.121	9.384	1.00 50.1	
ATOM ATOM	1980 1981	O M	THR		53 54	88.235	-6.305	8.452	1.00 48.6	
MION	T)01	И	ASP	Ð	54	87.175	-7.666	9.923	1.00 49.6	54 B

MOTA	1982	CA	ASP	В	54	85.836	-7.340	9.443	1.00 48.74	. В
MOTA	1983	CB	ASP	В	54	84.953	-8.602	9.442	1.00 47.27	
MOTA	1984	CG	ASP	В	54	85.315	-9.582	8.320	1.00 44.64	
MOTA	1985	OD1	ASP	В	54 ·	85.571	-9.119	7.190	1.00 46.93	
MOTA	1986	OD2	ASP	В	54	85.328	-10.811	8.560	1.00 39.85	
MOTA	1987	С	ASP	В	54	85.149	-6.226	10.237	1.00 46.99	
MOTA	1988	0	ASP	В	54	85.266	-6.157	11.460	1.00 41.92	
ATOM	1989	N	TYR	В	55	84.436	-5.365	9.509	1.00 50.33	
MOTA	1990	CA	TYR	В	55	83.691	-4.231	10.066	1.00 50.27	
ATOM	1991	CB	TYR	В	55	84.133	-2.928	9.401	1.00 53.07	
ATOM	1992	CG	TYR	В	55	85.608	-2.644	9.496	1.00 54.63	
ATOM	1993	CD1	TYR	В	55	86.317	-2.226	8.366	1.00 51.51	
MOTA	1994	CE1	TYR		55	87.678	-1.991	8.416	1.00 52.19	_
ATOM	1995	CD2	TYR		55 .	86.303	-2.815	10.700	1.00 52.89	
ATOM	1996	CE2	TYR	В	55	87.678	-2.578	10.767	1.00 58.41	
ATOM	1997	CZ	TYR	В	55	88.360	-2.168	9.611	1.00 56.38	
MOTA	1998	OH	TYR	В	55	89.721	-1.953	9.631	1.00 46.61	
MOTA	1999	C	TYR	В	55	82.189	-4.385	9.835	1.00 47.88	
MOTA	2000	0	TYR	\mathbf{B} .	55	81.719	-4.311	8.700	1.00 48.35	
ATOM	2001	N	VAL	В	56	81.444	-4.577	10.918	1.00 47.78	
MOTA	2002	CA	VAL	В	56	79.995	-4.728	10.846	1.00 45.91	
MOTA	2003	CB	VAL	В	56	79.541	-5.895	11.696	1.00 46.70	В
MOTA	2004	CG1	VAL	В	56	78.026	-6.004	11.664	1.00 50.38	В
MOTA	2005	CG2	VAL	В	56	80.179	-7.15 7	11.169	1.00 47.91	В
ATOM	2006	С	VAL	В	56	79.282	-3.463	11.302	1.00 44.29	В
ATOM	2007	0	VAL	В	56 .	79.582	-2.905	12.347	1.00 46.32	В
MOTA	2008	N	THR	В	57	78.298	-3.044	10.527	1.00 44.24	В
MOTA	2009	CA	THR		57	77.579	-1.810	10.802	1.00 41.17	В
MOTA	2010	CB	THR		57	78.069	-0.767	9.784	1.00 35.54	В
ATOM	2011	OG1	THR	В	57	78.063	0.536	10.353	1.00 38.40	В
MOTA	.2012	CG2	THR	B.	57	77.191	-0.784	8.572	1.00 27.33	В
ATOM	2013	C	THR		57	76.054	-1.990	10.654	1.00 41.10	В
ATOM	2014	0	THR		57	75.616	-2.869	9.914	1.00 41.91	В
ATOM	2015	N	LEU		58	75.252	-1.183	11.357	1.00 39.02	В
MOTA	2016	CA	LEU		58	73.798	-1.259	11.199	1.00 39.14	В
ATOM	2017	CB	LEU		58	73.052	-0.950	12.501	1.00 38.46	В
ATOM	2018	CG	LEU		58	71.522	-0.826	12.309	1.00 38.14	В
ATOM	2019		LEU		58	70.932	-2.186	11.924	1.00 32.30	В
ATOM	2020		LEU		58	70.862	-0.309	13.573	1.00 29.95	В
ATOM	2021	C	LEU		58	73.411	-0.219	10.140	1.00 40.92	В
ATOM	2022	0	LEU		58	72.990	0.892	10.471	1.00 45.82	В
ATOM	2023	N	GLN		59	73.565	-0.604	8.874	1.00 39.41	В
ATOM	2024	CA	GLN		59	73.283	0.226	7.702	1.00 39.53	В
ATOM	2025	CB	GLN		59	73.319	-0.659	6.450	1.00 45.44	В
MOTA MOTA	2026 2027	CG CD	GLN GLN		59 59	74.135	-0.146	5.275	1.00 54.90	В
ATOM	2027		GLM		59 59	73.755	1.253	4.850	1.00 63.38	В
ATOM	2028	NE2			59	74.192 72.930	2.239	5.450	1.00 70.49	В
ATOM	2029	C	GLN		59	72.930	1.351 0.960	3.815	1.00 67.26	В
MOTA	2030	0	GLN		59	71.863		7.747	1.00 38.18 1.00 35.51	В
ATOM	2032	И	ARG		60	70.877	2.156	7.486		В
MOTA	2032	CA	ARG		60	69.532	0.225	8.066 8.122	1.00 37.63 1.00 37.38	В
MOTA	2033	CB	ARG		60	68.953		6.704	1.00 37.38	В
MOTA	2034	CG	ARG		60	67.663	0.847 1.642	6.557	1.00 38.74	В
ATOM	2036	CD	ARG		60	67.105	1.553	5.135	1.00 45.15	В
MOTA	2037	NE	ARG		60	68.132	1.188	4.152	1.00 52.51	В
MOTA	2038	CZ	ARG		60	69.182	1.100	3.816	1.00 69.86	В
ATOM	2039		ARG		60	69.369	3.138	4.377	1.00 74.30	B B
				_	- 0	JJ.J	J. A.J.O	T.J//		₽ .

ATOM	2040	NH2	ARG	В	60	70.060	1.498	2.920	1.00 73.74	В
MOTA	2041	С	ARG	В	60	68.633	-0.076	9.023	1.00 38.91	В
ATOM	2042	0	ARG		60	68.877	-1.265	9.219	1.00 43.16	В
ATOM	2043	N	GLY		61	67.603	0.543	9.584	1.00 38.75	В
ATOM	2044	CA	GLY		61	66.677	-0.159	10.455	1.00 35.84	
ATOM	2045	C	GLY		61	65.320				В
							0.392	10.099	1.00 36.33	В
ATOM	2046	0	GLY		61	65.130	1.603	10.120	1.00 39.54	В
ATOM	2047	N	SER		62	64.376	-0.479	9.769	1.00 35.26	В
ATOM	2048	CA	SER		62	63.059	-0.022	9.368	1.00 33.15	В
ATOM	2049	CB	SER		62	62.901	-0.178	7.861	1.00 36.72	В
MOTA	2050	OG	SER		62	63.875	0.585	7.179	1.00 38.32	В
MOTA	2051	C	SER		62	61.942	-0.750	10.057	1.00 34.32	В
MOTA	2052	0	SER		62	62.029	-1.956	10.287	1.00 39.82	В
MOTA	2053	N	ALA		63	60.874	-0.011	10.344	1.00 32.23	В
MOTA	2054	CA	ALA	В	63	59.698	-0.551	11.027	1.00 31.25	В
ATOM	2055	CB	ALA	В	63	59.216	0.433	12.061	1.00 33.63	. B
MOTA	2056	C	ALA	В	63	58.559	-0.879	10.073	1.00 27.28	В
MOTA	2057	0	ALA	В	63	58.427	-0.264	9.030	1.00 26.51	В
MOTA	2058	N	TYR	В	64	57.736	-1.848	10.458	1.00 24.98	В
ATOM	2059	CA	TYR	В	64	56.600	-2.288	9.662	1.00 26.45	В
MOTA	2060	CB	TYR	В	64	56.973	-3.516	8.815	1.00 31.53	В
MOTA	2061	CG	TYR	В	64	58.009	-3.217	7.754	1.00 38.26	В
MOTA	2062	CD1	TYR	В	64	59.376	-3.266	8.043	1.00 39.16	В
MOTA	2063	CE1	TYR	В	64	60.322	-2.877	7.101	1.00 41.44	В
ATOM	2064	CD2	TYR	В	64	57.624	-2.784	6.494	1.00 36.50	В
MOTA	2065	CE2	TYR	В	64	58.555	-2.396	5.553	1.00 38.33	В
MOTA	2066	CZ	TYR	В	64	59.898	-2.437	5.856	1.00 44.74	В
ATOM	2067	OH	TYR		64	60.803	-2.007	4.914	1.00 50.52	В
ATOM	2068	C,	TYR		64	55.389	-2.630	10.519	1.00 26.87	В
ATOM	2069	oʻ	TYR		64	55.510	-2.908	11.716	1.00 25.93	В
MOTA	2070	Ŋ	GLY		65	54.219	-2.611	9.887	1.00 26.40	В
ATOM	2071	CA	GLY		65	52.986	-2.924	10.582	1.00 23.18	В
ATOM	2072	C	GLY		65	52.833	-2.159	11.877	1.00 27.39	В
ATOM	2073	ō	GLY		65	53.122	-0.948	11.965	1.00 27.74	В
ATOM	2074	N	GLY		66	52.393	-2.880	12.898	1.00 27.45	B
ATOM	2075	CA	GLY		66	52.172	-2.272	14.195	1.00 31.18	В
ATOM ·	2076	C	GLY		66	53.348	-1.484	14.709	1.00 29.93	В
ATOM	2077	ō	GLY		66	53.192	-0.363	15.161	1.00 33.78	B
ATOM	2078	N	VAL		67	54.533	-2.062	14.638	1.00 29.31	В
ATOM	2079	CA	VAL		67	55.701	-1.365	15.127	1.00 32.04	В
ATOM	2080	CB	VAL		67	56.983	-2.082	14.715	1.00 32.94	В
ATOM	2081		VAL		67	58.177	-1.150	14.915	1.00 26.67	В
ATOM	2082	CG2	VAL		67	57.149	-3.366	15.535	1.00 25.11	В
ATOM	2083	C.	VAL		67	55.769	0.052	14.607	1.00 33.57	В
ATOM	2084	ō	VAL		67	56.147	0.974	15.325	1.00 36.86	. B
ATOM	2085	N	LEU		68	55.379	0.212	13.356	1.00 35.52	В
ATOM	2086		LEU		68	55.417	1.496	12.672	1.00 37.28	В
ATOM	2087	СВ	LEU		68	55.311	1.226	11.176	1.00 36.92	В
ATOM	2088	CG	LEU		68	55.556	2.319	10.151	1.00 30.54	В
ATOM	2089		LEU		68	56.941	2.913	10.330	1.00 25.55	B
MOTA	2090		LEU		68	55.396	1.699	8.770	1.00 26.00	В
MOTA	2091	C	LEU		68	54.324	2.480	13.092	1.00 20.67	В
ATOM	2092		LEU		68	54.537	3.693	13.092	1.00 39.11	
ATOM	2092	N	SER		69	53.152	1.956	13.146	1.00 39.11	В
ATOM	2093	CA	SER		69	52.053	2.827	13.405	1.00 39.21	В
MOTA	2094	CB	SER		69	50.780	2.328	13.760	1.00 39.83	В
ATOM	2095	OG	SER		69	50.780	0.990			В
ATOM	2096	C	SER		69	51.785	2.996	13.474	1.00 39.64	B B
WT OLD	2021	·	بالتدب	L)		JI./03	4.330	15.237	1.00 39.99	•

MOTA	2098	0	SER	В	69	51.223	4.008	15.636	1.00 41.	46 B
MOTA	2099	N	ASN	В	70	52.187	2.018	16.046	1.00 38.	
MOTA	2100	CA	ASN		70	51.928	2.058	17.482	1.00 37.	
MOTA	2101	CB	ASN	В	70	51.219	0.772	17.900	1.00 35.	. –
ATOM	2102	CG	ASN		70	50.006	0.477	17.030	1.00 41.	
ATOM	2103		ASN		70	49.351	1.396	16.548	1.00 43.	
ATOM	2104		ASN	_	70	49.697	-0.802	16.830	1.00 42.	
ATOM	2105	C	ASN		70	53.110	2.286	18.412	1.00 40.	
ATOM	2106	ō	ASN		70	52.940	2.321	19.637	1.00 44.	
ATOM	2107	N	PHE		71	54.303	2.460	17.865	1.00 37.	
ATOM	2107	CA	PHE		71	55.438	2.624	18.747	1.00 37.	
ATOM	2109	CB	PHE		71	56.255	1.328	18.809	1.00 35.	
ATOM	2110	CG	PHE		71	55.520	0.159	19.394	1.00 20.	
ATOM	2111		PHE		71	54.585	-0.537	18.640	1.00 21.	
ATOM	2112	CD2	PHE		71	55.771	-0.258	20.711		
ATOM	2113	CE1			71	53.891	-0.258	19.198	1.00 15.	
ATOM	2113	CE2	PHE						1.00 35.	
MOTA	2114	CEZ	PHE		71 71	55.101 54.158	-1.356	21.275	1.00 15.	
							-2.064	20.524	1.00 21.	
MOTA MOTA	2116	C	PHE		71	56.371	3.745	18.359	1.00 38.	
	2117	0	PHE		71	56.329	4.259	17.235	1.00 38.	
MOTA	2118	N	SER		72	57.197	4.131	19.325	1.00 37.	
ATOM	2119	CA	SER		72	58.223	5.143	19.126	1.00 42.	
MOTA	2120	CB	SER		72	57.927	6.426	19.911	1.00 44.	
ATOM	2121	OG	SER		72	57.983	6.205	21.309	1.00 52.	
MOTA	2122	C	SER		72	59.403	4.408	19.732	1.00 42.	
MOTA	2123	0	SER		72	59.264	3.746	20.764	1.00 42.	
MOTA	2124	N	GLY		73	60.563	4.476	19.110	1.00 42.	
MOTA	2125	CA	GLY		73	61.629	3.717	19.717	1.00 45.	
MOTA	2126	C	GLY		73	63.039	3.995	19.301	1.00 43.	
MOTA	2127	0	GLY		73	63.311	4.815	18.414	1.00 40.	
ATOM	2128	И	THR		74	63.942	3.289	19.967	1.00 40.	
ATOM	2129	CA	THR		74	65.349	3.446	19.680	1.00 44.	
ATOM	2130	CB	THR		74	66.135	4.058	20.884	1.00 45.	
MOTA	2131		THR		74	66.173	3.116	21.965	1.00 49.	
MOTA	2132	CG2			74	65.482	5.355	21.353	1.00 36.	
ATOM	2133	C	THR		74	65.945	2.101	19.363	1.00 42.	
ATOM	2134	0	THR		74	65.336	1.056	19.615	1.00 36.	
MOTA	2135	N	VAL		75	67.138	2.146	18.783	1.00 45.	
MOTA	2136	CA	VAL		75	67.875	0.936	18.455	1.00 45.	
ATOM	2137	CB	VAL		75	68.138	0.786	16.915	1.00 46.	
MOTA	2138		VAL		75	68.889	2.013	16.355	1.00 40.	
ATOM	2139		VAL		75	68.919	-0.483	16.657	1.00 36.	
ATOM	2140	C ·	VAL		75	69.194	1.045	19.189	1.00 43.	
ATOM	2141	0	VAL		75	69.909	2.041	19.055	1.00 38.	
MOTA	2142	N	LYS		76	69.489	0.040	20.000	1.00 45.	
MOTA	2143	CA	LYS		76	70.743	0.029	20.732	1.00 49.	
MOTA	2144	CB	LYS		76	70.545	-0.495	22.159	1.00 53.	
MOTA	2145	CG.	LYS		76	71.714	-0.162	23.084	1.00 60.	
MOTA	2146	CD	LYS		76	71.479	-0.629	24.516	1.00 64.	
MOTA	2147	CE	LYS		76	72.622	-0.184	25.431	1.00 67.	
ATOM	2148	NZ	LYS		76	72.421	-0.608	26.851	1.00 72.	
MOTA	2149	C	LYS		76	71.741	-0.863	19.993	1.00 50.	
ATOM	2150	0	LYS		76	71.620	-2.091	20.011	1.00 50.	
MOTA	2151	N	TYR		77	72.717	-0.238	19.339	1.00 48.	
MOTA	2152	CA	TYR		77	73.734	-0.978	18.606	1.00 47.	
ATOM	2153	CB	TYR		77	73.890	-0.451	17.188	1.00 40.	
MOTA	2154	CG	TYR		77	74.855	-1.288	16.379	1.00 42.	46 B
MOTA	2155	CD1	TYR	В	77	74.661	-2.660	16.245	1.00 40.	68 B

MOTA	2156	CE1	TYR E	3 77	75.502	-3.431	15.462	1.00 44.37	В
ATOM	2157	CD2	TYR E		75.932	-0.709	15.712	1.00 44.07	В
ATOM	2158	CE2	TYR E		76.787	-1.467	14.919	1.00 39.44	В
ATOM	2159	CZ	TYR E		76.564	-2.833	14.789	1.00 48.45	В
ATOM	2160	OH	TYR E		77.347	-3.604	13.936	1.00 48.36	В
ATOM	2161	C	TYR E				19.242		
ATOM		_			75.108	-0.930		1.00 50.29	В
	2162	0	TYR E		75.811	0.070	19.116	1.00 52.49	В
ATOM	2163	N	SER B		75.503	-2.008	19.906	1.00 51.15	В
ATOM	2164	CA	SER E		76.827	-2.059	20.504	1.00 53.96	В
MOTA	2165	CB	SER B		77.892	-1.901	19.398	1.00 52.80	В
ATOM	2166	OG	SER B		79.223	-2.118	19.863	1.00 45.51	. В
ATOM	2167	C	SER B		77.022	-0.986	21.567	1.00 57.66	В
ATOM	2168	0	SER B		77.957	-0.191	21.488	1.00 61.05	В
ATOM	2169	N	GLY B	79	76.142	-0.947	22.558	1.00 59.91	В
ATOM	2170	CA	GLY B	79	76.301	0.044	23.609	1.00 60.98	· B
ATOM	2171	C	GLY B		75.660	1.407	23.410	1.00 61.44	В
MOTA	2172	0	GLY B	79	75.304	2.048	24.394	1.00 64.54	В
ATOM	2173	N	SER B	80	75.521	1.861	22.166	1.00 59.37	В
ATOM	2174	CA	SER B	80	74.908	3.164	21.888	1.00 58.61	В
ATOM	2175	CB	SER B	80	75.760	3.946	20.898	1.00 56.52	В
ATOM	2176	OG	SER B		76.995	4.272	21.491	1.00 65.42	В
ATOM	2177	C	SER B		73.480	3.061	21.347	1.00 57.58	Ŗ
ATOM	2178	ō	SER B		73.070	2.007	20.851	1.00 56.15	B
ATOM	2179	N	SER B		72.724	4.157	21.443	1.00 54.53	В.
ATOM	2180	CA	SER B		71.344	4.162	20.963	1.00 49.40	В
ATOM	2181	CB	SER B		70.356	4.417	22.110	1.00 51.39	В.
ATOM	2182	OG	SER B		69.796	3.204	22.597	1.00 31.39	В
ATOM	2183	C	SER B		71.102	5.162	19.852	1.00 47.28	
ATOM	2184	ō	SER B		71.765	6.192	19.747		В
								1.00 39.61	В
ATOM	2185	N	TYR B		70.152	4.826	18.996	1.00 45.93	В
ATOM	2186	CA	TYR B		69.830	5.688	17.880	1.00 46.60	В
ATOM	2187	CB	TYR B		70.613	5.268	16.616	1.00 49.73	B
ATOM	2188	CG	TYR B		72.093	5.009	16.838	1.00 51.38	В
ATOM	2189	CD1			72.528	3.887	17.552	1.00 49.31	В
ATOM	2190	CE1	TYR B		73.885	3.675	17.818	1.00 53.08	В
ATOM	2191	CD2	TYR B		73.057	5.911	16.383	1.00 55.97	В
ATOM	2192	CE2	TYR B		74.428	5.707	16.639	1.00 54.20	В
ATOM	2193	CZ	TYR B		74.831	4.590	17.360	1.00 56.12	В
ATOM	2194	OH	TYR B		76.171	4.388	17.625	1.00 59.66	В
ATOM	2195	C	TYR B		68.332	5.598	17.611	1.00 44.35	В
ATOM	2196	0	TYR B		67.644	4.643	18.024	1.00 40.57	В
ATOM	2197	N	PRO B	83	67.807	6.597	16.907	1.00 39.76	В
ATOM	2198	CD	PRO B		68.528	7.801	16.482	1.00 36.79	В
ATOM	2199	CA	PRO B	83	66.395	6.680	16.553	1.00 39.99	В
MOTA	2200	CB	PRO B	83	66.306	8.016	15.839	1.00 37.53	В
MOTA	2201	CG	PRO B	83	67.428	8.795	16.431	1.00 42.77	В
ATOM	2202	C	PRO B	83	65.984	5.535	15.642	1.00 41.79	В
ATOM	2203	0	PRO B	83	66.655	5.259	14.656	1.00 46.83	В
ATOM	2204	N	PHE B	84	64.889	4.868	15.975	1.00 41.27	В
ATOM	2205	CA	PHE B	84	64.381	3.779	15.146	1.00 41.36	В
MOTA	2206	CB	PHE B	84	64.508	2.440	15.866	1.00 37.32	В
MOTA	2207	CG	PHE B		63.949	1.288	15.089	1.00 34.18	В
MOTA	2208		PHE B		64.674	0.710	14.050	1.00 33.03	В
ATOM	2209		PHE B		62.683	0.789	15.383	1.00 31.71	В
ATOM	2210		PHE B		64.141	-0.355	13.316	1.00 36.61	В
MOTA	2211		PHE B		62.139	-0.333	14.655	1.00 38.81	В
ATOM	2212	CZ	PHE B		62.870	-0.852	13.621	1.00 31.68	В
ATOM	2213	C	PHE B		62.905	4.044	14.829	1.00 43.37	В
ALON	2213	•		. 5-2	52.303	4.044	14.023	~	Ð

	ATOM	2214	0	PHE	В	84	62.09	2	4.243	15.744	1.00	46.09	В
	ATOM	2215	N	PRO	В	85	62.52	5	4.016	13.533	1.00	41.86	В
	ATOM	2216	CD	PRO	В	85	61.11	.1	4.228	13.179	1.00	35.59	В
	ATOM	2217	CA	PRO	В	85	63.32	8	3.778	12.322	1.00	41.21	В
	ATOM	2218	CB	PRO		85	62.39		4.235	11.211		39.09	В
	ATOM	2219	CG	PRO		85	61.05		3.767	11.740		33.50	В
	ATOM	2220	C	PRO		85	64.63		4.543	12.337		39.65	В
	ATOM	2221	ō	PRO		85	64.69		5.638	12.873		43.24	В
	ATOM	2222	N	THR		86	65.68		3.973	11.757		36.93	
•	ATOM												В
		2223	CA	THR		86	66.98		4.626	11.750		38.77	В
	MOTA	2224	CB	THR		86	68.09		3.640	11.422		36.90	В
	ATOM	2225	_	THR		86	67.97		3.232	10.057		38.71	· B
	ATOM	2226	CG2	THR		86	68.00		2.424	12.322		39.15	В
	ATOM	2227	C	THR		86	67.04		5.752	10.744		43.31	В
	MOTA	2228	0	THR		86	66.25		5.794	9.802		43.75	В
	ATOM	2229	N	THR		87	67.99		6.658	10.942		50.06	В
	MOTA	2230	CA	THR		87	68.15		7.818	10.059		55.86	В
	MOTA	2231	CB	THR		87	67.81		9.115	10.800	1.00	54.71	В.
	MOTA	2232	OG1	THR		87	68.37		9.066	12.116	1.00	63.13	В
	ATOM	2233	CG2	THR	В	87	66.31		9.294	10.892	1.00	54.15	В
	ATOM	2234	C	THR	В	87	69.55		7.975	9.484	1.00	57.39	В
	MOTA	2235	0	THR	В	87	69.78	1	808.8	8.609	1.00	56.92	В
	ATOM	2236	N	SER	В	88	70.50		7.177	9.979	1.00	58.59	В
	MOTA	2237	CA	SER	В	88	71.87	8 '	7.238	9.506	1.00	58.12	В
	ATOM	2238	CB	SER	В	88	72.66		3.281	10.304	1.00	58.73	В
	MOTA	2239	OG	SER	В	88	72.92		7.819	11.620	1.00	60.37	В
	ATOM	2240	C	SER	В	88	72.55	5 !	5.887	9.681		57.61	В
	ATOM	2241	0	SER	В	88	72.13		5.078	10.509		55.11	В
	ATOM	2242	N	GLU		89	73.60		5.638	8.897		57.26	В
	ATOM	2243	CA	GLU		89	74.33		1.388	9.036		53.85	B .
	ATOM	2244	CB	GLU		89	75.27		1.132	7.857		56.12	В
	ATOM	2245	CG	GLU		89	76.36		3.104	8.177		54.43	В
	ATOM	2246	CD	GLU		89	76.99		2.504	6.946		54.39	В
	ATOM	2247		GLU		89	77.23		3.236	5.964		53.88	В
	ATOM	2248		GLU		89	77.27		1.293	6.972		53.17	В
	ATOM	2249	C	GLU		89	75.13		1.519	10.318		49.39	В
	ATOM	2250	ō	GLU		89	75.85		5.484	10.526		48.42	В
	ATOM	2251	N	THR		90	74.97		3.527	11.171		47.42	В
	MOTA		CA	THR		90	75.60		3.463	12.463		45.32	В
	MOTA	2253	CB	THR		90	75.02		2.285	13.230		44.31	В
	MOTA	2254		THR		90	74.77		2.685	14.573		48.38	В
	ATOM	2255		THR		90							
	ATOM	2256	C	THR		90	75.98		1.091	13.196		33.61	В
			0			90	77.12		3.318	12.400		47.66	В
	ATOM	2257	N	THR			77.68		3.089	11.335		46.49	В
	ATOM	2258		PRO		91	77.80		3.490	13.548		52.88	В
	ATOM	2259	CD	PRO		91	77.29			14.779		52.94	· B
•	ATOM	2260	CA	PRO		91	79.27		3.360	13.612		52.66	В
	MOTA	2261	CB	PRO		91	79.59		3.858	15.021		51.12	В
	ATOM	2262	CG	PRO		91	78.51		4.847	15.290		49.49	В
	ATOM	2263	C	PRO		91	79.61		1.880	13.419		51.26	В
	ATOM	2264	0	PRO		91	78.76		1.021	13.611		51.56	В
	MOTA	2265	N	ARG		92	80.86		1.580	13.069		52.78	В
	MOTA	2266	CA	ARG		92	81.27		0.193	12.826		54.30	В
	ATOM	2267	CB	ARG		92	82.21		0.126	11.607		59.45	В
	ATOM	2268	CG	ARG	В	92	83.50		0.923	11.716	1.00	66.71	В
	MOTA	2269	CD	ARG		92	84.42	4	0.665	10.506		68.78	В
	MOTA	2270	NE	ARG	В	92	85.80		1.161	10.672	1.00	73.17	В
	ATOM	2271	CZ	ARG		92	86.52	8	1.045	11.788	1.00	75.02	В

MOTA	2272	NH1	ARG	В	92	86.026	0.460	12.874	1.00 72.41	В
MOTA	2273	NH2	ARG	В	92	87.783	1.482	11.808	1.00 72.05	В
MOTA	2274	Ç	ARG	В	92	81.897	-0.602	13.972	1.00 50.97	В
MOTA	2275	0	ARG	В	92	82.780	-0.120	14.668	1.00 56.32	В
MOTA	2276	N	VAL	В	93 .	81.407	-1.826	14.154	1.00 45.19	В
MOTA	2277	CA	VAL		93	81.902	-2.756	15.166	1.00 40.21	В
ATOM	2278	СВ	VAL		93	80.769	-3.566	15.788	1.00 35.96	B
ATOM	2279		VAL		93	81.324	-4.588	16.762	1.00 29.73	В
ATOM	2280		VAL		93	79.810	-2.652	16.479		
•		C	VAL						1.00 43.00	В
ATOM	2281				93	82.818	-3.742	14.437	1.00 42.90	В
ATOM	2282	0	VAL		93.	82.619	-4.008	13.249	1.00 43.72	В
MOTA	2283	N	VAL		94	83.817	-4.295	15.125	1.00 43.31	В
MOTA	2284	CA	VAL		94	84.707	-5.225	14.439	1.00 42.65	В
MOTA	2285	CB	VAL		94	86.228	-4.848	14.547	1.00 41.03	В
MOTA	2286		VAL		94	86.417	-3.333	14.428	1.00 40.89	В
MOTA	2287		VAL		94	86.834	-5.421	15.803	1.00 31.28	В
ATOM	2288	C	VAL		94	84.572	-6.659	14.879	1.00 44.53	В
MOTA	2289	0	VAL	В	94	84.361	-6.962	16.058	1.00 41.27	В
MOTA	2290	N	TYR	В	95	84.691	-7.533	13.885	1.00 47.17	В
MOTA	2291	CA	TYR	В	95	84.623	-8.967	14.074	1.00 47.30	В
ATOM	2292	CB	TYR	B	- 95	83.506	-9.570	13.206	1.00 44.54	В
MOTA	2293 .	CG	TYR	В	95	82.139	-9.360	13.793	1.00 40.07	В
MOTA	2294	CD1	TYR	В	95	81.574	-8.095	13.838	1.00 36.98	В
MOTA	2295	CE1	TYR	В	95	80.379	-7.876	14.478	1.00 35.11	В
ATOM	2296	CD2	TYR	В	95	81.454	-10.411	14.402	1.00 42.29	В
ATOM	2297	CE2	TYR		95	80.250	-10.198	15.050	1.00 41.04	В
ATOM		CZ	TYR		95	79.724	-8.924	15.085	1.00 40.92	В
ATOM	2299	OH	TYR		95	78.544	-8.686	15.750	1.00 52.81	В
ATOM	2300	C	TYR		95	85.983	-9.522	13.665	1.00 46.53	В
ATOM	2301	ō ·	TYR		95	86.452	-9.291	12.537	1.00 47.03	В
MOTA	2302	N	ASN		96		-10.241	14.595	1.00 40.40	В
MOTA	2303	CA	ASN		96		-10.836	14.373	1.00 36.00	В
MOTA	2304	CB	ASN		96	88.991	-9.949	14.954		
MOTA	2305	CG	ASN		96		-9.275	16.215	1.00 37.54	В
						88.544			1.00 42.61	В
MOTA	2306		ASN		96	88.215	-8.089	16.201	1.00 54.86	В
MOTA	2307		ASN		96		-10.023	17.314	1.00 37.56	В
ATOM	2308	C	ASN		96		-12.196	15.016	1.00 36.16	В
MOTA	2309	0	ASN		96		-12.408	15.890	1.00 38.38	В
ATOM	2310	N	SER		97		-13.130	14.584	1.00 33.66	В
MOTA	2311	CA	SER		97		-14.463	15.128	1.00 30.79	В
MOTA	2312	CB	SER		97		-14.460		1.00 16.62	В
MOTA	2313	OG	SER		97		-15.746	16.987	1.00 28.93	В
MOTA	2314	C	SER		97		-15.369	14.339	1.00 34.93	В
MOTA	2315	0	SER		97	85.294	-14.949	13.893	1.00 34.96	В
MOTA	2316	N	ARG		98	86.791	-16.607	14.138	1.00 38.81	В
MOTA	2317	CA	ARG	В	98		-17.559	13.407	1.00 40.04	В
MOTA	2318	CB	ARG		98	86.818	-18.786	13.016	1.00 43.35	В
ATOM	2319	CG	ARG	В	98	87.890	-18.522	11.967	1.00 53.22	В
ATOM	2320	$^{\rm CD}$	ARG	В	98	88.492	-19.832	11.428	1.00 61.19	В
MOTA	2321	NE	ARG	В	98.	89.443	-19.604	10.336	1.00 69.42	В
MOTA	2322	CZ	ARG	В	98	90.657	-19.071	10.484	1.00 71.95	В
MOTA	2323	NH1	ARG	В	98		-18.705	11.688	1.00 69.75	В
MOTA	2324		ARG		98		-18.888	9.421	1.00 72.04	В
ATOM	2325	С	ARG		98		-17.962	14.338	1.00 43.19	В
ATOM	2326	ō	ARG		98		-18.616	13.925	1.00 46.97	В
ATOM	2327	N	THR		99		-17.566	15.601	1.00 43.07	В
ATOM	2328	CA	THR		99		-17.896	16.575	1.00 47.92	В
ATOM	2329	CB	THR		99		-17.757	17.998	1.00 47.92	В
MION	2,2,	CD	T 111/	٠		07.7/4	11.151	11.000	1.00 40.09	Ð

								Q	
MOTA	2330	OG1	THR I	3 99	85.720	-18.441	18.117	1.00 51.61	В
MOTA	2331	CG2	THR I		83.483	-18.366	18.966	1.00 46.02	В
MOTA	2332	C	THR I	3 99	82.735	-16.981	16.426	1.00 50.30	В
ATOM	2333	0	THR I		82.873	-15.750	16.367	1.00 50.66	В
ATOM	2334	N	ASP I	3 100	81.548	-17.584	16.373	1.00 48.39	В
MOTA	2335	CA	ASP I		80.318	-16.818	16.232	1.00 50.11	В
MOTA	2336	CB	ASP I	3 100	79.098	-17.731	16.138	1.00 52.94	В
MOTA	2337	CG	ASP I	3 100	78.890	-18.305	14.753	1.00 58.51	В
MOTA	2338	OD1	ASP I	3 100	79.199	-17.617	13.749	1.00 55.67	В
MOTA	2339	QD2	ASP I		78.387	-19.447	14.676	1.00 61.45	В
MOTA	2340	C	ASP I	3 100	80.088	-15.863	17.386	1.00 49.54	В
MOTA	2341	0	ASP I	3 100	79.821	-16.281	18.504	1.00 49.52	В
ATOM	2342	N	LYS I	3 1 01	80.190	-14.576	17.090	1.00 51.30	В
MOTA	2343	CA	LYS I	3 101	79.964	-13.513	18.055	1.00 49.68	В
ATOM	2344	CB	LYS I	3 101	81.015	-12.417	17.872	1.00 52.75	В
MOTA	2345	CG	LYS I	3 101	80.670	-11.081	18.506	1.00 59.69	В
MOTA	2346	$^{\rm CD}$	LYS I	3 101	81.785	-10.068	18.294	1.00 58.80	В
MOTA	2347	CE	LYS I		81.469	-8.748	18.963	1.00 60.08	В
ATOM	2348	NZ	LYS I	3 101	82.634	-7.847	18.820	1.00 61.72	В
MOTA	2349	С	LYS I	3 101	78.570	-12.970	17.737	1.00 47.59	В
MOTA	2350	0	LYS I	3 101	78.088	-13.114	16.615	1.00 44.10	В
MOTA	2351	N	PRO I	3 102	77.893	-12.359	18.726	1.00 48.05	В
MOTA	2352	CD	PRO I	3 102	78.126	-12.429	20.175	1.00 46.67	В
MOTA	2353	CA	PRO I	3 102	76.553	-11.823	18.467	1.00 46.05	В
ATOM	2354	CB	PRO I	3 102	75.963	-11.650	19.874	1.00 44.50	В
ATOM	2355	CG	PRO I	3 102	76.722	-12.638	20.692	1.00 46.71	В
MOTA	2356	C	PRO I	3 102	76.614	-10.501	17.723	1.00 40.70	В
ATOM	2357	0		3 102	77.658		17.647	1.00 39.82	В
ATOM .	2358	N	TRP I	3 103	75.491	-10.117	17.144	1.00 37.30	В
ATOM	2359	CA	TRP E		75.389	-8.843	16.452	1.00 35.99	В
MOTA	2360	CB	TRP F		74.681	-9.064	15.119	1.00 30.34	В
MOTA	2361	CG	TRP I		74.579	-7.851	14.277	1.00 31.38	В
ATOM	2362	CD2	TRP E		73.422	-7.404	13.562	1.00 30.61	В
ATOM	2363	CE2	TRP E		73.783		12.886	1.00 23.58	В
MOTA	2364	CE3	TRP F		72.111		13.430	1.00 31.21	В
MOTA	2365		TRP I			-6.942	14.012	1.00 29.45	В
MOTA	2366		TRP I		75.097		13.176	1.00 26.89	В
MOTA	2367	CZ2	TRP I		72.884		12.089	1.00 19.17	В
ATOM	2368		TRP I		71.224		12.637	1.00 29.96	В
ATOM	2369	CH2	TRP I		71.620		11.979	1.00 23.18	В
ATOM	2370	C	TRP I		74.529		17.483	1.00 36.03	В
MOTA	2371	0		3 103	73.307		17.575	1.00 35.89	В
ATOM	2372	N		3 104	75.184		18.298	1.00 34.03	В
ATOM	2373	CD		3 104	76.553		17.988	1.00 36.29	В
MOTA	2374	CA		3 104	74.608		19.362	1.00 30.77	В
ATOM	2375	CB		3 104	75.842			1.00 25.97	В
ATOM	2376	CG	PRO I		76.697		18.838	1.00 26.96	В
MOTA	2377	C		3 104	73.606		18.885	1.00 30.38	В
MOTA	2378	0		3 104	73.921		18.755	1.00 30.99	В
ATOM	2379	N	VAL		72.394		18.626	1.00 28.53	В
ATOM	2380	CA		3 105	71.322		18.169	1.00 26.24	В
MOTA	2381	CB	VAL I		70.972		16.679	1.00 26.56 1.00 23.98	В
ATOM	2382		VAL I		69.944		16.231		В
MOTA	2383		VAL I		72.198		15.823	1.00 24.94	В
ATOM	2384	C		3 105	70.098		18.978	1.00 28.16	В
MOTA	2385	0		3 105	69.786		19.175	1.00 22.10 1.00 32.05	В
MOTA	2386	N		3 106	69.418		19.465		В
ATOM	2387	CA	ALA I	70 <i>p</i>	68.194	-4.499	20.224	1.00 34.01	В

MOTA	2388	CB	ALA B	106	68.482	-4.598	21.688	1.00 31.60	В
MOTA	2389	C	ALA B	106	67.265	-3.334	19.952	1.00 38.42	В
ATOM	2390	0	ALA B		67.703	-2.180	19.834	1.00 39.67	В
MOTA	2391	N	LEU B		65.983	-3.666	19.820	1.00 39.39	. В
MOTA	2392	CA	LEU B		64.931	-2.695	19.573	1.00 39.55	В
MOTA	2393	CB	LEU B		63.905	-3.276	18.602	1.00 37.52	В
MOTA	2394	CG	LEU B		63.970	-2.848	17.132	1.00 36.22	В
ATOM	2395		LEU B		65.387	-2.593	16.687	1.00 35.01	В
MOTA	2396	CD2			63.319	-3.905	16.296	1.00 27.15	В
ATOM	2397	C	LEU B		64.258	-2.406	20.896	1.00 39.73	В
ATOM	2398	0	LEU B		63.900	-3.327	21.624	1.00 41.16	В
ATOM	2399	N	TYR B		64.132	-1.126	21.221	1.00 42.11	В
ATOM	2400	CA	TYR B		63.462	-0.693	22.445	1.00 43.26	В
ATOM ATOM	2401 2402	CB CG	TYR B		64.375 65.357	.0.203	23.280	1.00 42.36	В
ATOM	2402		TYR B		66.634	-0.595 -0.860	24.086 23.601	1.00 48.99 1.00 58.34	B B
ATOM	2404		TYR B		67.524	-1.667	24.313	1.00 63.83	В
ATOM	2405		TYR B		64.986	-1.152	25.306	1.00 51.96	В
ATOM	2406	CE2	TYR B		65.858	-1.961	26.027	1.00 59.54	В
ATOM	2407	CZ	TYR B		67.131	-2.219	25.527	1.00 65.06	В
ATOM	2408	OH	TYR B		68.010	-3.027	26.230	1.00 69.27	В
ATOM	2409	C	TYR B		62.224	0.060	21.977	1.00 41.89	В
ATOM	2410	O	TYR B		62.312	1.191	21.492	1.00 41.81	В
ATOM	2411	N	LEU B	109	61.075	-0.592	22.113	1.00 39.72	В
ATOM	2412	CA	LEU B	109	59.827	-0.025	21.635	1.00 43.02	В
MOTA	2413	CB	LEU B	109	59.212	-0.982	20.610	1.00 39.34	В
MOTA	2414	CG	LEU B	109	60.170	-1.497	19.534	1.00 36.17	В
ATOM	2415	CD1	LEU B	109	59.463	-2.491	18.626	1.00 31.98	В
ATOM	2416		LEU B		60.710	-0.334	18.744	1.00 20.51	В
MOTA	2417	C	LEU B		58.804	0.266	22.719	1.00 44.10	В
ATOM	2418	0	LEU B		58.481	-0.617	23.512	1.00 43.98	В
ATOM	2419	N	THR B		58.291	1.500	22.728	1.00 43.50	В
ATOM	2420	CA	THR B		57.282	1.933	23.695	1.00 41.99	В
MOTA	2421	CB	THR B		57.740	3.163	24.481	1.00 44.49	В
ATOM	2422	OG1			59.001	2.891	25.096	1.00 53.82	В
ATOM ATOM	2423	CG2 C	THR B		56.729	3.503 2.288	25.569 22.998	1.00 48.58	В
ATOM	2424 2425	0	THR B		55.976 55.935	3.168	22.123	1.00 40.09 1.00 37.35	B B
MOTA	2425	N	PRO B		54.883	1.616	23.389	1.00 37.33	В
ATOM	2427	CD	PRO B		54.781	0.584	24.433	1.00 41.24	В
ATOM	2428	CA	PRO B		53.570	1.869	22.789	1.00 43.07	В
ATOM	2429	CB	PRO B		52.651	0.878	23.515	1.00 43.27	В
ATOM	2430	CG	PRO B		53.570	-0.203	23.970	1.00 42.12	В
ATOM	2431	C	PRO B	111	53.132	3.302	23.005	1.00 41.16	В
ATOM	2432	0	PRO B		53.493	3.927	24.009	1.00 39.11	В
ATOM	2433	N	VAL B	112	52.367	3.819	22.053	1.00 41.94	В
ATOM	2434	CA	VAL B	112	51.857	5.176	22.155	1.00 45.88	В
ATOM	2435	CB	VAL B	112	51.658	5.823	20.767	1.00 47.57	В
MOTA	2436	CG1	VAL B	112	53.013	6.036	20.097	1.00 43.97	В
MOTA	2437	CG2	VAL B	112	50.745	4.950	19.907	1.00 36.70	В
MOTA	2438	C	VAL B		50.521	5.112	22.869	1.00 48.87	В
MOTA	2439	0	VAL B		49.854	4.075	22.862	1.00 50.84	В
ATOM	2440	N	SER B		50.134	6.216	23.494	1.00 53.12	В
MOTA	2441	CA	SER B		48.869	6.264	24.221	1.00 55.18	В
MOTA	2442	CB	SER B		48.601	7.685	24.711	1.00 56.10	В
ATOM	2443	OG	SER B		48.456	8.567	23.614	1.00 56.76	В
ATOM	2444	C	SER B		47.696	5.801	23.364	1.00 53.23	В
ATOM	2445	0	SER B	113	46.718	5.264	23.879	1.00 53.63	В

MOTA	2446	N	SER 1	3 114	47.802	6.003	22.056	1.00 48.75	В
MOTA	2447	CA	SER 1	3 114	46.729	5.628	21.154	1.00 46.92	В
ATOM	2448	CB	SER I	3 114	46.755		19.920	1.00 48.64	В
ATOM	2449	OG	SER I	3 114	47.935		19.158	1.00 50.05	В
ATOM	2450	C		3 114	46.753		20.731	1.00 46.39	В
ATOM	2451	ō		3 114	45.871		20.014	1.00 44.89	В
ATOM	2452	N		3 115	47.757				
ATOM	2453	CA		3 115	47.879		21.185	1.00 49.38	В
ATOM	2454	CB		3 115			20.834	1.00 53.40	В
MOTA					49.116		21.497	1.00 56.78	B
	2455	C		3 115	46.634		21.226	1.00 54.70	В
ATOM	2456	0	ALA I		46.232		22.400	1.00 48.97	. В
ATOM	2457	N		3 116	46.049		20.236	1.00 56.98	В
MOTA	2458	CA	GLY I		44.853		20.461	1.00 57.50	В
MOTA	2459	C		3 116	44.944		21.530	1.00 54.48	В
MOTA	2460	0	GLY I		45.205	-1.090	22.710	1.00 53.95	В
ATOM	2461	N	GLY I	3 117	44.677	-2.581	21.113	1.00 50.75	В
ATOM	2462	CA	GLY I	3 117	44.757	-3.714	22.015	1.00 49.30	В
ATOM	2463	C	GLY I	3 117	45.923	-4.506	21.459	1.00 45.39	В
ATOM	2464	0	GLY F	3 117	46.970	-4.621	22.101	1.00 43.18	В
ATOM	2465	N	VAL I	3 118	45.730	-5.031	20.249	1.00 40.82	В
ATOM	2466	CA	VAL E	118	46.761	-5.775	19.539	1.00 38.09	В
ATOM	2467	CB	VAL E	118	46.141	-6.759	18.560	1.00 36.33	В
ATOM	2468	CG1	VAL E		47.195	-7.255	17.577	1.00 27.83	В
ATOM	2469		VAL E		45.525	-7.910	19.331	1.00 33.81	В
ATOM	2470	c	VAL E		47.599	-4.782	18.739	1.00 35.81	В
ATOM	2471	ŏ	VAL E		47.210	-4.404	17.652	1.00 38.24	
ATOM	2472	N	ALA E		48.739	-4.357	19.272		В
ATOM	2473	CA	ALA E			-3.405		1.00 32.10	В
ATOM	2474	CB	ALA E		49.586		18.570	1.00 28.90	В
ATOM	2475	C			50.362	-2.597	19.560	1.00 28.57	В
			ALA E		50.551	-4.052	17.566	1.00 32.45	В
ATOM	2476	.0	ALA E		51.188	-3.348	16.789	1.00 33.60	В
MOTA	2477	N	ILE E		50.677	-5.379	17.613	1.00 31.08	В
ATOM	2478	CA	ILE E		51.532	-6.129	16.703	1.00 30.88	В
ATOM	2479	CB	ILE E		52.918	-6.352	17.301	1.00 35.81	В
MOTA	2480	CG2			53.721	-7.282	16.411	1.00 27.80	В
ATOM	2481		ILE E		53.648	-5.024	17.460	1.00 36.87	В
MOTA	2482		ILE E		54.991	~5.165	18.133	1.00 38.89	В
MOTA	2483	C	ILE E	120	50.914	-7.511	16.418	1.00 35.91	В
MOTA	2484	0	ILE E	120	50.741	-8.321	17.334	1.00 40.23	В
MOTA	2485	N	LYS E	121	50.587	-7.789	15.161	1.00 30.56	В
MOTA	2486	CA	LYS E	121	49.998	-9.073	14.830	1.00 35.75	В
MOTA	2487	CB	LYS E	121	49.273	-9.010	13.473	1.00 44.54	В
MOTA	2488	CG	LYS E	121	47.826	~8.530	13.481	1.00 49.90	В
MOTA	2489.	CD	LYS E	121	47.721	-7.060	13.872	1.00 62.79	В
MOTA	2490	CE	LYS E	121	46.366	~6.495	13.487	1.00 65.42	В
ATOM	2491	NZ	LYS E	121	46.120	-6.665	12.020	1.00 68.24	. B
MOTA	2492	С	LYS E		50.966	-10.266	14.798	1.00 35.90	В
ATOM	2493	0	LYS E			-10.174	14.368	1.00 33.23	В
MOTA	2494	N	ALA E			-11.399	15.261	1.00 34.06	В
ATOM	2495	CA	ALA E			-12.625	15.247	1.00 33.24	В
ATOM	2496	CB	ALA E			-13.749	15.848	1.00 15.20	В
MOTA	2497	C	ALA E			-12.910	13.764	1.00 35.26	
ATOM	2498	ō	ALA E			-12.866	12.931	1.00 35.26	В
ATOM	2499	И	GLY E			-13.180	13.446	1.00 35.27	В
ATOM	2500	CA	GLY E						В
ATOM	2501	CA				-13.491	12.081	1.00 33.01	В
ATOM			GLY E			-12.307	11.195	1.00 33.84	В
	2502	0	GLY E	_		-12.482	10.024	1.00 33.30	В
ATOM	2503	N	SER E	124	53.434	-11.102	11.744	1.00 32.53	В

MOTA	2504	CA	SER I	3 124	53.704	-9.921	10.937	1.00 32.72	В
MOTA	2505	CB	SER I	3 124	52.839	-8.745	11.432	1.00 31.20	В
MOTA	2506	OG	SER I	3 124	53.032	-8.452	12.802	1.00 24.03	В
MOTA	2507	C	SER I		55.161	-9.467	10.816	1.00 34.32	В
ATOM	2508	0	SER E	3 124	56.003	-9.733	11.678	1.00 36.98	В
MOTA	2509	N	LEU E	3 125	55.451	-8.776	9.723	1.00 32.72	В
MOTA	2510	ĊA	LEU I	3 125	56.785	-8.261	9.519	1.00 29.75	В
ATOM	2511	CB	LEU E		56.994	-7.753	8.083	1.00 27.40	В
MOTA	2512	CG	LEU E		58.322	-7.004	7.913	1.00 27.74	В
MOTA	2513	CD1			59.482	-7.956	8.153	1.00 20.32	В
ATOM	2514		LEU F		58.402	-6.394	6.539	1.00 26.43	В
ATOM	2515	C	LEU E		56.836	-7.108	10.476	1.00 26.95	В
MOTA	2516	0	LEU E		56.099	-6.138		1.00 32.13	В
ATOM	2517	N	ILE E		57.718	-7.219	11.437	1.00 29.14	В
ATOM	2518	CA	ILE E		57.857	-6.192	12.445	1.00 31.84	В
ATOM ATOM	2519	CB CG2	ILE E		58.036	-6.876	13.812	1.00 34.18	В
ATOM	2520 2521	CG2	ILE E		59.342	-6.498	14.466	1.00 23.70	В
ATOM	2521	CD1	ILE E		56.810 56.827	-6.606 -7.374	14.653	1.00 30.98	В
ATOM	2523	CDI	ILE E		58.986	-5.234	15.923 12.140	1.00 49.29	В
ATOM	2524	0	ILE E		58.887	-4.060	12.140	1.00 32.54 1.00 31.40	В
ATOM	2525	N	ALA E		60.048	-5.730	11.501	1.00 31.40	В
ATOM	2526	CA	ALA E		61.197	-4.887	11.169	1.00 32.48	B B
ATOM	2527	CB	ALA E		61.970	-4.546	12.436	1.00 30.49	В
ATOM	2528	C	ALA E		62.156	-5.508	10.159	1.00 27.91	В
ATOM	2529	Ŏ	ALA E		62.198	-6.727	9.988	1.00 32.60	В
ATOM	2530	N	VAL E		62.915	-4.656	9.482	1.00 19.26	В
ATOM	2531	CA	VAL E		63.912	-5.126	8.540	1.00 19.14	В
ATOM	2532	CB	VAL E		63.572	-4.760	7.071	1.00 14.82	В
ATOM	2533	CG1	VAL E		64.768	-5.061	6.178	1.00 14.77	В
ATOM	2534	CG2	VAL E	128	62.386	-5.580	6.577	1.00 13.30	В
MOTA	2535	C	VAL E	128	65.226	-4.446	8.949	1.00 22.98	В
ATOM	2536	Ο.	VAL E	128	65.305	-3.220	9.003	1.00 27.09	В
MOTA	2537	N	LEU E		66.246	-5.240	9.255	1.00 21.47	В
MOTA	2538	CA	LEU E		67.531	-4.699	9.676	1.00 24.76	В
ATOM	2539	CB	LEU E		67.909	-5.233	11.055	1.00 26.80	В
ATOM	2540	CG	LEU E		66.928	-4.908	12.184	1.00 33.18	В
MOTA	2541		LEU E		67.450	-5.505	13.458	1.00 28.58	В
ATOM	2542		LEU E		66.759	-3.393	12.341	1.00 30.83	В
ATOM	2543	C	LEU B		68.633	-5.046	8.696	1.00 29.03	В
MOTA	2544	0	LEU B		68.858	-6.218	8.374	1.00 31.02	В
MOTA	2545	N	ILE E		69.335	-4.021	8.229	1.00 27.82	В
ATOM	2546	CA	ILE E		70.404	-4.231	7.271	1.00 28.56	, B
ATOM ATOM	2547 2548	CB CG2	ILE B		70.310	-3.256	6.082	1.00 28.77	В
ATOM	2549	-	ILE B		71.511	-3.443	5.163	1.00 23.87	В
ATOM	2550		ILE B		69.019	-3.525	5.301	1.00 23.15	В
ATOM ·	2551	CDI	ILE B		68.79 1 71.782	-2.534 -4.123	4.190 7.883	1.00 33.95 1.00 30.91	В
ATOM	2552	ō	ILE B		72.198	-3.063	8.366	1.00 30.91	В
ATOM	2553	N	LEU B		72.198	-5.253	7.841	1.00 31.82	В
ATOM	2554	CA	LEU B		73.817	-5.392	8.363	1.00 32.57	В
ATOM	2555	СВ	LEU B		73.989	-6.793	8.937	1.00 27.43	В
ATOM	2556	CG	LEU B		75.339	-7.075	9.589	1.00 27.43	В
ATOM	2557		LEU B		75.207	-8.278	10.512	1.00 35.23	B B
ATOM	2558		LEU B		76.396	-7.297	8.517	1.00 32.03	В
ATOM	2559	C	LEU B		74.762	-5.180	7.203	1.00 30.34	В
MOTA	2560	ō	LEU B		74.672	-5.874	6.205	1.00 30.34	В
MOTA	2561	N	ARG B		75.668	-4.216	7.335	1.00 33.58	В

ATOM	2562	CA	ARG I	3 132	76.636	-3.918	6.281	1.00 32.72	В
MOTA	2563	CB	ARG I	3 132	76.558	-2.450	5.910	1.00 29.90	В
MOTA	2564	CG	ARG I	3 132	77.554	-2.020	4.892	1.00 24.57	В
ATOM	2565	CD	ARG I	3 132	77.230	-0.618	4.505	1.00 28.98	В
ATOM	2566	NE	ARG 1	3 132	77.771	-0.263	3.202	1.00 44.88	В
MOTA	2567	CZ	ARG I	3 132	77.466	0.863	2.558	1.00 52.26	В
MOTA	2568	NH1	ARG I	3 132	76.623	1.738	3.106	1.00 53.41	В
ATOM	2569	NH2	ARG I	3 132	77.996	1.118	1.364	1.00 49.10	В
ATOM	2570	C	ARG I	3 132	78.041	-4.261	6.749	1.00 34.78	В
ATOM	2571	0	ARG I	3 132	78.522	-3.720	7.749	1.00 36.33	В
MOTA	2572	N	GLN F	3 133	78.697	-5.154	6.009	1.00 35.46	В
ATOM	2573	CA	GLN I	3 133	80.033	-5.627	6.352	1.00 31.37	В
ATOM	2574	CB	GLN I	3 133	79.981	-7.127	6.635	1.00 31.04	B
MOTA	2575	CG	GLN F	3 133	81.331	-7.809	6.828	1.00 38.48	В
ATOM	2576	CD	GLN F	3 133	81.903	-8.404	5.549	1.00 37.23	В
ATOM	2577	OE1	GLN I	3 133	81.262	-9.204	4.870	1.00 41.88	В
MOTA	2578	NE2	GLN F	3 133	83.121	-8.020	5.225	1.00 38.07	В
MOTA	2579	C	GLN F	133	81.082	-5.351	5.297	1.00 33.10	В
ATOM	2580	0	GLN E	133	80.913	-5.684	4.120	1.00 32.79	В
ATOM	2581	N	THR E	134	82.168	-4.728	5.742	1.00 32.27	В
ATOM	2582	CA	THR E	134	83.312	-4.405	4.902	1.00 31.08	В
MOTA	2583	CB	THR E	134	83.485	-2.913	4.787	1.00 28.44	В
ATOM	2584	OG1	THR E	134	83.318	-2.351	6.092	1.00 43.54	В
MOTA	2585	CG2	THR E	134	82.477	-2.318	3.827	1.00 17.92	В
ATOM	2586	C	THR E	134	84.552	-4.973	5.605	1.00 34.91	В
ATOM	2587	0	THR E	134	84.439	-5.789	6.526	1.00 .31.52	В
MOTA	2588	N	ASN E		85.739	-4.553	5.180	1.00 38.08	В
ATOM	2589	CA .	ASN E	135	'86.948	-5.058	5.817	1.00 43.90	В
MOTA	2590	CB	ASN E	135	87.226	-6.490	5.364	1.00 43.43	В
MOTA	2591	CG	ASN E	135	87.306	-6.602	3.862	1.00 45.83	В
MOTA	2592	OD1	ASN E	135	87.848	-5.719	3.199	1.00 38.68	В
MOTA	2593	ND2	ASN E	135	86.764	-7.684	3.313	1.00 47.13	В
ATOM	2594	C	ASN E	135	88.153	-4.199	5.506	1.00 46.43	В
ATOM	2595	0	ASN E	135	88.082	-3.278	4.686	1.00 48.60	В
ATOM	2596	N	ASN E		89.261	-4.504	6.174	1.00 47.15	В
ATOM	2597	CA	ASN E		90.512	-3.785	5.954	1.00 49.23	В
MOTA	2598	CB	ASN E		91.279	-3.636	7.257	1.00 49.84	В
ATOM	2599	. CG	ASN E		91.594	-4.972	7.899	1.00 53.73	В
ATOM	2600		ASN E		92.152	~5.029	8.995	1.00 55.74	В
MOTA	2601		ASN E		91.234	-6.057	7.223	1.00 55.06	В
ATOM	2602	C	ASN E		91.362	-4.584	4.992	1.00 51.02	В
ATOM	2603	0	ASN E		92.576	-4.634	5.137	1.00 50.25	В
MOTA	2604	N	TYR E		90.718	-5.232	4.026	1.00 55.30	В
ATOM	2605	CA	TYR E		91.440	-6.042	3.060	1.00 55.24	В
ATOM	2606	CB	TYR E		91.152	-7.527	3.263	1.00 62.18	В
ATOM	2607	CG	TYR E		91.947	-8.398	2.315	1.00 73.43	В
ATOM	2608		TYR E		93.341	-8.310	2.258	1.00 71.51	В
ATOM	2609		TYR E		94.075	-9.093	1.374	1.00 75.13	В
ATOM	2610		TYR E		91.306	-9.299	1.457	1.00 78.65	В
ATOM	2611		TYR E			-10.091	0.567	1.00 77.61	В
ATOM	2612	CZ	TYR E		93.415	-9.980	0.534	1.00 76.38	В
ATOM	2613	OH	TYR E			-10.755	-0.343	1.00 75.82	В
MOTA	2614	C	TYR E		91.163	-5.680	1.619	1.00 53.40	В
MOTA	2615	0	TYR E		92.084	-5.650	0.819	1.00 58.08	В
ATOM	2616	N	ASN B		89.909	-5.406	1.276	1.00 50.33	В
MOTA	2617	CA	ASN E		89.578	-5.040	-0.099	1.00 48.93	В
MOTA	2618	CB	ASN B		89.458	-6.282	-0.961	1.00 51.42	В
MOTA	2619	CG	ASN B	T38	88.427	-7.245	-0.448	1.00 52.18	В

A'	TOM	2620	OD1	ASN I	B 13	38	88.288	-8.334	-0.980	1.00 57.78	В
A'	TOM	2621	ND2	ASN 1	B 1:	38	87.696	-6.855	0.586	1.00 52.16	В
	TOM	2622	C	ASN			88.304	-4.228	-0.224	1.00 51.07	В
	TOM	2623	ō	ASN I			87.829	-3.656	0.757	1.00 53.81	В
	TOM	2624	И	SER :			87.740	-4.180	-1.427		
										1.00 51.10	В
	TOM	2625	CA	SER I			86.518	-3.398	-1.642	1.00 51.76	В
_	TOM	2626	CB	SER I			86.478	-2.854	-3.080	1.00 51.64	В
A.	TOM	2627	OG	SER I			86.441	-3.906	-4.029	1.00 59.56	В
A	TOM	2628	С	SER 1			85.201	-4.124	-1.333	1.00 45.24	В
A.	MOT	2629	0	SER 1	3 13	39	84.141	-3.711	-1.805	1.00 42.38	В
A'	TOM	2630	N	ASP 1	3 14	40	85.272	-5.193	-0.543	1.00 42.97	В
A.	TOM	2631	CA	ASP 1	3 14	40	84.083	-5.957	-0.165	1.00 42.60	В
	TOM	2632	СВ	ASP I			84.482	-7.220	0.624	1.00 40.34	B
	TOM	2633	CG	ASP I			84.912	-8.376	-0.284	1.00 41.15	В
	TOM	2634		ASP I			85.331	-9.441	0.233	1.00 30.91	·B
	TOM	2635		ASP I			84.826	-8.223	-1.524	1.00 34.85	_
				ASP I							В
	TOM	2636	C				83.100	-5.113	0.665	1.00 45.06	В
	TOM	2637	0	ASP I			83.428	-4.609	1.741	1.00 44.68	В
	TOM	2638	N	ASP I			81.888	-4.966	0.149	1.00 45.88	. В
A.	IOM	2639	CA	ASP I			80.838	-4.208	0.819	1.00 42.51	В
A.	TOM	2640	CB	ASP 1	3 14	41	80.690	-2.844	0.152	1.00 47.71	. В
A'	TOM	2641	CG	ASP I	3 14	41	79.889	-1.863	0.984	1.00 52.18	В
· A	MOT	2642	OD1	ASP I	3 14	41	79.089	-2.289	1.849	1.00 53.12	В
A'	TOM	2643	OD2	ASP 1	3 14	41	80.051	-0.650	0.753	1.00 56.00	В
	TOM	2644	C	ASP I			79.558	-5.027	0.616	1.00 39.58	В
	TOM	2645	ō	ASP I			78.849	-4.840	-0.375	1.00 39.26	В
	rom	2646	N	PHE I			79.272	-5.931	1.546	1.00 32.52	·B
	TOM	2647	CA	PHE I			78.107	-6.799	1.429	1.00.32.32	
											В
	TOM	2648	CB	PHE I			78.520	-8.261	1.648	1.00 33.39	В
	TOM	2649	CG	PHE I			79.576	-8.747	0.694	1.00 36.64	В
	TOM	2650		PHE I			80.722	-9.387	1.168	1.00 40.51	В
	TOM	2651	CD2	PHE 1			79.411	-8.609	-0.682	1.00 33.21	В
A.	TOM	2652	CE1	PHE 1	3 14	12	81.687	-9.890	0.282	1.00 33.95	В
A.	TOM	2653	CE2	PHE 1			80.361	-9.104	-1.564	1.00 31.13	В
A'	TOM	2654	cz	PHE 1	3 14	12	81.504	-9.749	-1.078	1.00 30.25	В
A.	TOM	2655	С	PHE 1	3 14	12	77.011	-6.445	2.420	1.00 35.53	В
A'	MOT	2656	0	PHE I	3 14	12	77.270	-5.894	3.495	1.00 38.43	В
	TOM	2657	N	GLN I			75.778	-6.780	2.063	1.00 33.86	В
	TOM	2658	CA	GLN I			74.652	-6.491	2.934	1.00 30.03	В
	TOM	2659	СВ	GLN I			73.656	-5.581	2.245	1.00 28.31	В
	TOM	2660	CG	GLN I			74.140			1.00 28.31	
		2661	CD	GLN I				-4.193	1.953		В
	TOM						72.987	-3.292	1.625	1.00 42.93	В
	TOM	2662	OE1				72.083	-3.685	0.886	1.00 44.79	В
	TOM	2663	NE2	GLN I			72.998	-2.075	2.175	1.00 48.07	В
	TOM	2664	C	GLN 1			73.934	-7.751	3.351	1.00 29.96	В
A.	MOI	2665	0	GLM 1			73.617	-8.602	2.523	1.00 28.85	В
A'	TOM	2666	N	PHE 1	3 14	14	73.696	-7.865	4.650	1.00 30.75	В
A.	TOM	2667	CA	PHE 1	3 14	14	73.006	-9.002	5.220	1.00 28.73	В
A'	TOM	2668	CB	PHE 1	3 14	44	73.823	-9.602	6.358	1.00 26.51	В
	TOM	2669	CG	PHE 1	3 14	14		-10.278	5.897	1.00 30.21	В
	TOM	2670		PHE			76.129	-9.543	5.350	1.00 29.83	В
	TOM	2671		PHE I				-11.667	6.004	1.00 23.03	В
	TOM			PHE I							
		2672						-10.187	4.917	1.00 24.03	В
	TOM	2673		PHE I				-12.313	5.577	1.00 25.07	В
	TOM	2674	CZ	PHE 1				-11.567	5.034	1.00 22.57	В
	TOM	2675	C	PHE I			71.689	-8.451	5.720	1.00 30.12	В
	TOM	2676	0	PHE 1			71.647	-7.697	6.697	1.00 32.53	В
A'	rom	2677	N	VAL 1	3 14	45	70.611	-8.834	5.043	1.00 26.21	В

MOTA	2678	CA	VAL E	145	69.298	-8.345	5.391	1.00 24.86	В
ATOM	2679	CB	VAL B	145	68.484	-8.083	4.119	1.00 27.44	В
ATOM	2680	CG1	VAL B	145	67.112	-7.586	4.481	1.00 22.84	В
ATOM	2681	CG2			69.215	-7.059	3.230	1.00 23.64	В
ATOM	2682	C	VAL B		68.524	-9.268	6.296	1.00 27.22	В
ATOM		ō							
	2683		VAL B		68.301		5.964	1.00 33.37	В
MOTA	2684	N	TRP B		68.101	-8.751	7.444	1.00 28.51	В
MOTA	2685	CA	TRP B		67.332	-9.550	8.396	1.00 26.43	В
MOTA	2686	CB	TRP B	146	67.969	-9.459	9.788	1.00 23.18	В
MOTA	2687	CG	TRP B	146	69.457	-9.701	9.755	1.00 23.47	В
ATOM ~	2688	CD2	TRP B	146	70.124	-10.968	9.730	1.00 19.01	В
MOTA	2689	CE2	TRP B	146	71.508		9.603	1.00 22.45	В
MOTA	2690	CE3	TRP B	146	69.687		9.797	1.00 20.35	В
ATOM	2691		TRP B		70.433	-8.756	9.648	1.00 24.85	В
ATOM	2692		TRP B			-9.352	9.552	1.00 28.21	В
ATOM	2693				72.462				
							9.546	1.00 19.23	В
ATOM	2694		TRP B	•	70.645		9.735	1.00 18.67	В
ATOM	2695	CH2			72.012		9.612	1.00 14.89	В
MOTA	2696	C	TRP B		65.872	-9.084	8.436	1.00 27.93	В
ATOM	2697	0	TRP B		65.578	-7.915	8.682	1.00 30.75	В
MOTA	2698	N	ASN B	147	64.957	-10.002	8.157	1.00 25.92	В
MOTA	2699	CA	ASN B	147	63.535	-9.683	8.176	1.00 23.01	В
ATOM .	2700	CB	ASN B	147	62.825	-10.307	6.961	1.00 21.04	В
MOTA	2701	CG	ASN B	147	63.425	-9.849	5.632	1.00 25.61	В
ATOM	2702		ASN B		63.616	-8.654		1.00 22.73	В
ATOM	2703		ASN B		63.718		4.768	1.00 29.40	В
ATOM	2704	C	ASN B		62.978		9.477	1.00 25.03	В
ATOM	2705	0	ASN B		62.851		9.653	1.00 27.78	В
ATOM	2706	N	ILE B		62.657	-9.315	10.394	1.00 21.98	В
ATOM	2707	CA	ILE B		62.156	-9.697	11.713	1.00 23.38	В
ATOM	2708	CB	ILE B		62.529	-8.625	12.772	1.00 24.49	В
MOTA	2709		ILE B		62.482	-9.241	14.163	1.00 20.09	В
MOTA	2710	CG1	ILE B	148	63.892	-7.990	12.443	1.00 26.37	В
MOTA	2711	CD1	ILE B	148	65.094	-8.922	12.458	1.00 18.27	В
MOTA	2712	C	ILE B	148	60.646	-9.892	11.779	1.00 24.19	В
MOTA	2713	0	ILE B	148	59.894	-8.939	11.623	1.00 31.82	В
ATOM	2714	\mathbf{N}_{i}	TYR B	149	60.198		12.013	1.00 22.13	В
ATOM	2715	CA	TYR B		58.768		12.131	1.00 26.16	В
ATOM	2716	CB	TYR B		58.359		11.272	1.00 24.29	В
ATOM	2717	CG	TYR B		58.323		9.789	1.00 31.59	В
MOTA	2718		TYR B		59.506		9.036	1.00 31.39	
									В
ATOM	2719		TYR B		59.473		7.678	1.00 30.53	. В
ATOM	2720		TYR B		57.106		9.133	1.00 32.75	В
MOTA	2721		TYR B		57.063		7.772	1.00 30.71	В
ATOM	2722	CZ	TYR B		58.246		7.052	1.00 36.24	В
MOTA	2723	OH	TYR B	149	58.194		5.705	1.00 42.36	В
ATOM	2724	C	TYR B	149	58.400	-11.673	13.589	1.00 30.29	В
MOTA	2725	0	TYR B	149	59.185	-12.282	14.318	1.00 34.87	В
MOTA	2726	N	ALA B	150	57.217	-11.245	14.021	1.00 30.88	В
MOTA	2727	CA	ALA B	150	56.768		15.385	1.00 31.72	В
ATOM	2728	СВ	ALA B		55.968		15.913	1.00 27.66	В
ATOM	2729	C	ALA B		55.917		15.351	1.00 32.87	В
MOTA		Ö	ALA B		55.029				
	2730						14.513	1.00 33.67	В
ATOM	2731	N	ASN B		56.182		16.264	1.00 31.00	В
ATOM	2732	CA	ASN B		55.452		16.287	1.00 32.71	В
MOTA	2733	CB	ASN B		56.261		17.006	1.00 37.45	В
MOTA	2734	CG	ASN B		57.406		16.175	1.00 36.34	В
MOTA	2735	OD1	ASN B	151	57.213	-17.075	15.061	1.00 40.47	В

ATOM	2736	ND2	ASN I	3 151	58.605	-16.526	16.721	1.00 39.04	В
ATOM	2737	С		3 151		-14.883	16.970	1.00 32.85	В
ATOM	2738	0	ASN I	3 151		-15.732	16.781	1.00 37.18	В
ATOM	2739	N	ASN I	3 152		-13.839	17.763	1.00 31.83	В
ATOM	2740	CA	ASN I			-13.682	18.519	1.00 31.46	В
ATOM	2741	CB	ASN I			-14.178	19.931	1.00 31.71	В
ATOM	2742	CG	ASN I			-13.325	20.663	1.00 33.57	В
ATOM	2743		ASN I			-13.400	20.406	1.00 39.77	В
ATOM	2744	ND2	ASN I			-12.492	21.569	1.00 33.77	
ATOM	2745	C	ASN I			-12.244			В
ATOM	2746	ō	ASN I			-11.309	18.600 18.274	1.00 31.23 1.00 21.68	В
ATOM	2747	N	ASP I			-12.083	19.065		В
MOTA	2748	CA	ASP I			-10.753		1.00 33.06	В
ATOM	2749	CB	ASP I			-10.785	19.228 19.481	1.00 35.00	В
ATOM	2749	CG	ASP I			-11.399	18.343	1.00 35.22	В
ATOM	2751		ASP I			-11.402		1.00 40.27	В
ATOM	2751		ASP I			-11.402	17.176	1.00 42.01	В
ATOM		C	ASP I				18.629	1.00 35.56	В
	2753					-10.082	20.455	1.00 35.09	В
MOTA	2754	0	ASP I			-10.728	21.466	1.00 36.89	В
ATOM	2755	N	VAL E		51.297	-8.789	20.346	1.00 34.31	. В
MOTA	2756	CA	VAL E		51.764	-8.002	21.466	1.00 31.02	В
MOTA	2757	CB	VAL E		52.986	-7.195	21.123	1.00 31.01	В
ATOM	2758			3 154 ·	53.320	-6.251	22.288	1.00 28.37	В
ATOM ATOM	2759 2760	CG2	VAL E		54.121	-8.112	20.836	1.00 38.21	. В
ATOM	2760	C	VAL E		50.615	-7.022	21.783	1.00 33.12	В
ATOM	2762	N O	VAL E		50.396 49.871	-6.032	21.070	1.00 32.38	. В
ATOM	2762	CA	VAL E				22.836	1.00 33.40	В
ATOM	2764	CB	VAL E		48.756 47.671	-6.487 -7.315	23.269 24.026	1.00 33.75	В
ATOM	2765		VAL E		46.746	-6.387		1.00 33.02	В
ATOM	2766		VAL E			-8.159	24.779	1.00 35.87	В
ATOM	2767	C	VAL E		49.183	-5.362	23.049	1.00 35.78	В
ATOM	2768	õ	VAL E		50.005	-5.559	24.203 25.098	1.00 32.16 1.00 31.88	В
ATOM	2769	N	VAL E		48.618	-4.183	23.982	1.00 35.48	B B
ATOM	2770	CA	VAL E		48.866	-3.020	24.838	1.00 38.42	В
ATOM	2771	CB	VAL E		49.272	-1.792	24.024	1.00 40.77	В
ATOM	2772	CG1			49.178	-0.546	24.898	1.00 35.57	В
ATOM	2773		VAL E		50.691	-1.976	23.471	1.00 40.94	В.
ATOM	2774	C	VAL E		47.523	-2.731	25.502	1.00 38.00	В
ATOM	2775	ō	VAL E		46.608	-2.225	24.860	1.00 40.60	В.
ATOM	2776	N	PRO E		47.387	-3.046	26.795	1.00 38.40	В
ATOM	2777	CD	PRO E		48.444	-3.501	27.705	1.00 40.01	В
MOTA	2778	CA	PRO E		46.135	-2.824	27.533	1.00 39.19	В
ATOM	2779	CB	PRO E		46.504	-3.192	28.967	1.00 38.60	В
ATOM	2780	CG	PRO E		47.642	-4.173	28.778	1.00 42.51	В
MOTA	2781	C	PRO E		45.595	-1.410	27.428	1.00 35.87	В
ATOM	2782	0	PRO E		46.362	-0.436	27.385	1.00 34.12	В
ATOM	2783	N	THR E		44.273	-1.301	27.359	1.00 33.32	В
ATOM	2784	CA	THR E		43.655	0.013	27.282	1.00 38.28	В
MOTA	2785	CB	THR E		42.204	-0.080	26.822	1.00 42.15	В
ATOM	2786	OG1			41.587	1.203	26.977	1.00 50.48	В
MOTA	2787	CG2			41.453	-1.089	27.648	1.00 46.98	В
ATOM	2788	С	THR E		43.705	0.682	28.666	1.00 37.13	В
ATOM	2789	0		3 158	43.429	0.039	29.686	1.00 34.91	В
MOTA	2790	N	GLY E		44.077	1.965	28.690	1.00 35.68	В
ATOM	2791	CA	GLY E		44.171	2.700	29.943	1.00 35.75	В
ATOM	2792	C	GLY E		42.882	3.368	30.418	1.00 37.79	В
ATOM	2793	0	GLY E		41.823	3,254	29.777	1.00 37.36	В
						. — —	·		_

MOTA	2794	N	GLY F	3 160		42.951	4.051	31.557	1.00 32.85	В
MOTA	2795	CA	GLY I	3 160		41.764	4.714	32.049	1.00 33.30	В
ATOM	2796	С	GLY E			41.701	6.073	31.402	1.00 34.94	В
ATOM	2797	0	GLY F			42.698	6.513	30.841	1.00 35.86	В
ATOM	2798	N	CYS I			40.558	6.749	31.477	1.00 35.19	В
ATOM	2799	CA	CYS I			40.436	8.073	30.875	1.00 37.82	В
ATOM	2800	C	CYS I			40.898	9.209	31.799	1.00 37.82	
ATOM	2801	ŏ	CYS I			41.193	8.982	32.976	1.00 43.89	В
MOTA	2802	CB	CYS I			39.006	8.286	30.460		В
ATOM	2802	SG	CYS I			38.372	6.895	29.480	1.00 37.49	В
ATOM	2804	N	ASP I			40.997	10.426	31.269	1.00 44.87	В
ATOM	2805	CA	ASP I			41.421			1.00 39.46	В
ATOM	2806	CB	ASP I			42.589	11.541 12.307	32.102 31.481	1.00 44.50	В
ATOM	2807	CG	ASP I			43.226	13.285		1.00 50.21	В
ATOM	2808		ASP I			43.513	12.877	32.468 33.619	1.00 63.52 1.00 65.05	В
ATOM	2809		ASP I			43.444	14.462	32.102		В
ATOM	2810	C	ASP I			40.257	12.474	32.336	1.00 70.61	В
ATOM	2811	Ö	ASP I			39.556	12.869	31.406	1.00 47.74 1.00 49.17	В
ATOM	2812	N	VAL E			40.043	12.810	33.596		В
ATOM	2813	CA	VAL E			38.948	13.674	33.959	1.00 49.77	В
ATOM	2814	CB	VAL E			38.235	13.134	35.201	1.00 55.00	В
ATOM	2815		VAL E			37.114	14.062	35.611	1.00 53.21 1.00 52.34	В
ATOM	2816	CG2				37.688	11.735	34.900	1.00 52.34	В
MOTA	2817	C	VAL E			39.463	15.073	34.196	1.00 52.49	В
MOTA	2818	Ö	VAL E			39.759	15.472	35.314	1.00 65.20	В
ATOM	2819	N	SER E			39.568	15.809	33.101	1.00 65.20	B B
ATOM	2820	CA	SER E			40.044	17.179	33.101	1.00 72.84	
ATOM	2821	CB	SER E			40.125	17.688	31.656	1.00 84.26	B B
ATOM	2822	OG	SER E			40.585		30.770	1.00 84.26	В
ATOM	2823	C	SER E			39.100	18.067	33.910	1.00 85.96	В
ATOM	2824	ō	SER E			37.965	18.331	33.488	1.00 86.73	В
ATOM	2825	N	ALA E			39.576	18.520	35.068	1.00 89.66	В
MOTA	2826	CA	ALA E			38.797	19.393	35.948	1.00 94.00	В
ATOM	2827	CB	ALA E			38.319	18.616	37.168	1.00 91.90	В
ATOM	2828	C	ALA E			39.654	20.582	36.386	1.00 96.86	В
ATOM	2829	ō	ALA E			40.808	20.407	36.786	1.00100.35	В
ATOM	2830	N	ARG E			39.098	21.789	36.306	1.00100.33	В
ATOM	2831	CA	ARG E		:	39.838	22.985	36.693	1.00 98.96	В
ATOM	2832	CB	ARG E			38.986	24.221	36.417	1.00 93.90	В.
ATOM	2833	CG	ARG E			38.598	24.315	34.949	1.00 96.82	В
ATOM	2834	CD	ARG E			37.840	25.588	34.607	1.00 99.58	В
ATOM	2835	NE	ARG E			37.445	25.608	33.195	1.00101.53	В
ATOM	2836	CZ	ARG E			36.640	26.515	32.644	1.00100.65	В
ATOM	2837		ARG E			36.134	27.494	33.385	1.00 97.72	В
ATOM	2838		ARG E			36.329	26.434	31.353	1.00 98.46	В
ATOM	2839	C	ARG E			40.307	22.926	38.154	1.00101.70	В
ATOM	2840	ō	ARG E			41.518	22.859	38.396	1.00104.32	В
ATOM	2841	N	ASP E			39.375	22.949	39.114	1.00101.24	В
MOTA	2842	CA	ASP E			39.712	22.852	40.549	1.00101.61	В
ATOM	2843	CB	ASP E			40.814	23.842	40.945	1.00105.04	В
ATOM	2844	CG	ASP E			41.305	23.632	42.383	1.00108.69	В
ATOM	2845		ASP E			42.020	24.515	42.904	1.00103.03	В
ATOM	2846		ASP E			40.976	22.586	42.995	1.00106.87	В
ATOM	2847	C	ASP E			38.527	23.064	41.489	1.00100.64	В
ATOM	2848	ō	ASP E			37.380	22.826	41.115	1.00103.25	В
MOTA	2849	N	VAL E			38.833	23.502	42.712	1.00103.23	В
ATOM	2850	CA	VAL E			37.853	23.772	43.762	1.00 91.56	В
ATOM	2851	CB	VAL E			38.570	24.071	45.101	1.00 92.06	В
						20.0,0	~~ ~ ~ ~ ~ ~ ~		22.00	L.

ATOM	2852	CG1	VAL	В	168	39.670	25.090	44.878	1.00	93.27	В
ATOM	2853	CG2	VAL	В	168	37.576	24.586	46.130	1.00	91.17	В
ATOM	2854	С	VAL	В	168	36.945	24.947	43.390	1.00	85.88	В
MOTA	2855	0	VAL	В	168	37.229	26.101	43.708	1.00	85.97	В
ATOM	2856	N	THR	В	169	35.846	24.628	42.717	1.00	79.23	В
ATOM	2857	CA	THR			34.885	25.618	42.267		77.03	В
ATOM	2858	CB	THR			33.730	24.955	41.502		76.80	В
ATOM	2859	OG1	THR		169	34.212	24.463	40.249		80.08	В
ATOM	2860	CG2	THR			32.612	25.948	41.247		75.39	В
ATOM	2861	C	THR			34.286	26.455	43.372		76.63	В
ATOM	2862	Ö	THR		169		.25.929	44.350	1.00	76.32	В
ATOM	2863	N	VAL			34.363	27.769	43.195		77.34	
ATOM	2864	CA	VAL			33.804	28.707	44.156		78.44	В
ATOM	2865	CB	VAL			34.483	30.099	44.156		81.17	В
ATOM	2866	CG1	VAL		170	33.967					В
ATOM		CG2	VAL			35.996	30.995	45.171 44.180		82.29	В
	2867		VAL .				29.961			83.39	В
ATOM	2868	C	VAL		170	32.317	28.855	43.840		77.18	В
ATOM	2869	0	THR			31.927	29.605	42.948		71.35	В
ATOM	2870	N				31.500	28.092	44.558		81.19	В
ATOM	2871	CA	THR			30.056	28.122	44.395		84.05	. В
ATOM	2872	CB	THR			29.391	26.887	45.087		82.25	В
ATOM	2873	OG1				27.969	27.043	45.102		86.37	В
ATOM	2874	CG2	THR			29.862	26.743	46.512		79.27	В
ATOM	2875	C	THR			29.595	29.408	45.063		87.98	В
MOTA	2876	0	THR			28.578	29.438	45.755		92.17	В
MOTA	2877	N	LEU			30.353	30.476	44.839		89.17	В
ATOM	2878	CA	LEU			30.056	31.763	45.446		92.60	В
MOTA	2879	CB	LEU			31.237	32.733	45.245		96.55	В
MOTA	2880	CG	LEU		172	31.432	33.924	46.208		98.54	В
MOTA	2881		LEU			32.839	34.495	46.034		98.01	В
MOTA	2882		LEU			30.388	35.004	45.953		98.92	В
MOTA	2883	С	LEU			28.753	32.431	45.007		92.79	В
ATOM	2884	0	LEU			28.174	33.174	45.792	1.00	94.65	В
ATOM	2885	N	PRO		173	28.264	32.175	43.773	1.00	90.85	В
ATOM	2886	CD	PRO	B :	173	28.521	31.050	42.860	1.00	88.96	В
ATOM	2887	CA	PRO			27.008	32.847	43.403	1.00	90.43	В
MOTA	2888	CB	PRO	В	173	26.503	32.015	42.218	1.00	88.69	В
MOTA	2889	CG	PRO	В	173	27.124	30.675	42.445	1.00	89.49	В
ATOM	2890	С	PRO	В	173	26.047	32.844	44.588	1.00	90.40	В
MOTA	2891	0	PRO	В	173	25.250	31.920	44.750	1.00	93.67	В
MOTA	2892	N	ASP			26.149	33.890	45.408	1.00	86.06	В
ATOM	2893	·CA	ASP	В	174	25.366	34.043	46.627	1.00	81.80	В
MOTA	2894	CB	ASP	В	174	25.137	35.525	46.902	1.00	85.92	В
MOTA	2895	CG	ASP	В	174	26.441	36.267	47.139	1.00	88.15	В
MOTA	2896	OD1	ASP	В	174	27.202	36.459	46.164	1.00	86.99	В
MOTA	2897	OD2	ASP	В	174	26.716	36.640	48.303		94.90	. в
MOTA	2898	С	ASP	В	174	24.069	33.256	46.666	1.00	77.31	В
ATOM	2899	0	ASP	В	174	23.344	33.169	45.676	1.00	73.43	В
MOTA	2900	N	TYR	В	175	23.806	32.687	47.837	1.00	74.04	В
MOTA	2901	CA	TYR	В	175	22.662	31.822	48.075	1.00	74.02	В
MOTA	2902	CB	TYR	В	175	21.768	32.337	49.199	1.00	70.97	В
MOTA	2903	CG	TYR			20.473	31.551	49.222		68.59	В
MOTA	2904		TYR			20.482	30.171	49.416	1.00	65.93	В
ATOM	2905		TYR			19.318	29.423	49.306		66.29	В
ATOM	2906	CD2	TYR			19.257	32.160	48.928		67.00	В
ATOM	2907	CE2	TYR			18.087	31.417	48.819		65.36	В
ATOM	2908	CZ	TYR			18.127	30.052	49.008		63.55	В
MOTA	2909	OH	TYR			16.975	29.321	48.898		64.36	В
				_							_

ATOM	2910	С	TYR E	3 175	21.750	31.428	46.917	1.00 75.18	В
MOTA	2911	0	TYR F	3 175	21.519	30.243	46.695	1.00 83.24	В
ATOM	2912	N	PRO I		21.183	32.392	46.186	1.00 67.87	В
		CD	PRO I		20.952	33.833	46.386		В
MOTA	2913							1.00 60.03	
MOTA	2914	CA	PRO I		20.331	31.854	45.120	1.00 62.12	В
MOTA	2915	CB	PRO I	3 176	19.365	32.998	44.866	1.00 62.04	В
ATOM	2916	CG	PRO E	3 176	20.253	34.208	45.109	1.00 66.57	В
MOTA	2917	С	PRO F	176	21.062	31.406	43.848	1.00 57.47	В
ATOM	2918	ō	PRO I		20.572	30.547	43.108	1.00 52.79	В
ATOM	2919	N	GLY I		22.238	31.987	43.619	1.00 56.05	В
MOTA	2920	CA	GLY I		23.030	31.701	42.429	1.00 57.16	В
MOTA	2921	С	GLY I		23.447	30.275	42.097	1.00 57.68	В
MOTA	2922	0	GLY F	3 177	23.498	29.406	42.968	1.00 61.93	, B
MOTA	2923 ·	N	SER E	3 178	23.767	30.047	40.824	1.00 52.24	В
MOTA	2924	CA	SER E	3 178	24.184	28.740	40.354	1.00 48.46	В
MOTA	2925	CB	SER E	3 178	22.983	27.979	39.791	1.00 45.43	В
ATOM	2926	OG	SER I		22.709	28.358	38.449	1.00 39.13	В
ATOM	2927	C	SER I		25.237	28.891	39.264	1.00 50.58	В
ATOM	2928	0	SER I		25.073	29.696	38.350	1.00 53.44	В
MOTA	2929	N	VAL E		26.317	28.119	39.349	1.00 51.43	В
ATOM	2930	CA	VAL I	3 179	27.360	28.202	38.331	1.00 51.70	В
MOTA	2931	CB	VAL E	3 179	28.774	28.442	38.919	1.00 46.82	В
ATOM	2932	CG1	VAL E	3 179	28.733	29.466	40.009	1.00 50.97	В
MOTA	2933	CG2	VAL E	3 179	29.339	27.141	39.438	1.00 52.80	В
ATOM	2934	C	VAL E		27.461	26.905	37.556	1.00 52.92	В
ATOM	2935	ō	VAL I		26.909	25.874	37.957	1.00 51.89	B
ATOM	2936	N	PRO E		28.153	26.951	36.408	1.00 54.24	В
ATOM	2937	CD	PRO I		28.525	28.164	35.661	1.00 49.71	В
MOTA	2938	CA	PRO I	3 180	28.346	25.760	35.578	1.00 51.83	В
MOTA	2939	CB	PRO E	3 180	28.542	26.340	34.185	1.00 49.00	В
ATOM	2940	CG	PRO E	3 180	29.273	27.590	34.475	1.00 51.54	В
MOTA	2941	С	PRO E	3 180	29.616	25.135	36.151	1.00 47.16	В
ATOM	2942	ō	PRO E		30.450	25.839	36.730	1.00 41.66	· B
MOTA	2943	N	ILE E		29.736	23.819	36.032	1.00 47.39	В
MOTA	2944	CA	ILE E		30.892	23.108	36.559	1.00 43.01	В
ATOM	2945	CB	ILE E		30.487	21.975	37.493	1.00 44.32	В
MOTA	2946		ILE E		31.731	21.348	38.073	1.00 50.39	В
MOTA	2947	CG1	ILE E	3 181	29.609	22.510	38.622	1.00 46.67	В
MOTA	2948	CD1	ILE E	3 181	29.108	21.449	39.572	1.00 44.10	В
ATOM	2949	С	ILE H	3 181	31.714	22.512	35.446	1.00 42.62	В
ATOM	2950	0	ILE E		31.323	21.529	34.795	1.00 35.02	В
ATOM	2951	N	PRO I		32.883	23.104	35.208	1.00 47.08	В
MOTA	2952	CD	PRO I		33.468	24.243	35.932	1.00 46.65	В
			PRO I						В
ATOM	2953	CA			33.782	22.631	34.157	1.00 45.30	
MOTA	2954	CB	PRO I		34.902	23.665	34.164	1.00 49.60	В
MOTA	2955	CG	PRO I		34.278	24.882	34.860	1.00 48.89	· B
MOTA	2956	C	PRO 1	3 182	34.293	21.259	34.535	1.00 44.84	В
ATOM	2957	0	PRO I	3 182	34.974	21.098	35.552	1.00 41.12	В
MOTA	2958	N	LEU I	3 183	33.933	20.268	33.732	1.00 46.51	В
ATOM	2959	CA	LEU I		34.382	18.909	33.966	1.00 47.25	В
ATOM	2960	CB	LEU I		33.616	18.268	35.132	1.00 50.90	B
			LEU I				35.132	1.00 30.90	B
ATOM	2961	CG			34.309	17.147			
MOTA	2962		LEU I		33.434	16.714	37.089	1.00 46.65	В
ATOM	2963		LEU 1		34.588	15.972	35.019	1.00 52.20	В
MOTA	2964	C	LEU 1		34.155	18.124	32.687	1.00 48.27	В
MOTA	2965	0	LEU I	3 183	33.021	17.901	32.253	1.00 47.09	В
MOTA	2966	N	THR 1	3 184	35.260	17.724	32.075	1.00 51.78	В
MOTA	2967	CA		3 184	35.224	16.959	30.840	1.00 50.01	В
									_

ATOM	2968	CB	THR	В	184	35.779	17.784	29.677	1.00	51.81	. В
ATOM	2969	OG1	THR	В	184	37.008	18.404	30.086	1.00	54.34	В
ATOM	2970	CG2	THR	В	184	34.777	18.853	29.250	1.00	49.61	В
ATOM	2971	С	THR	В	184	36.089	15.723	31.017	1.00	47.48	В
ATOM	2972	0	THR	В	184	36.862	15.626	31.970		43.70	В
ATOM	2973	N			185	35.935	14.773	30.106		45.69	В
ATOM	2974	CA			185	36.720	13.558	30.146		48.55	B
ATOM	2975	CB			185	35.950	12.367	30.778		49.34	В
MOTA	2976		VAL			35.650	12.659	32.207		57.28	В
ATOM	2977		VAL			34.662		30.015			
			VAL				12.091			46.09	В
MOTA	2978	C				37.078	13.160	28.735		49.59	В
ATOM	2979	0			185	36.259	13.295	27.815		47.94	В
ATOM	2980	N			186	38.306	12.687	28.559		48.79	В
ATOM	2981	CA			186	38.727	12.214	27.256		50.15	В
MOTA	2982	CB			186	39.636	13.221	26.548		46.07	В
MOTA	2983	CG			186	40.908		27.265		52.19	В
ATOM	2984		TYR			42.060	12.759	27.016		59.11	B
ATOM	2985		TYR			43.242	13.008	27.714		63.38	В
ATOM	2986		TYR			40.964	14.515	28.224	1.00	61.62	В
MOTA	2987	CE2	TYR			42.143	14.777	28.932	1.00	64.92	В
MOTA	2988	CZ			186	43.274	14.019	28.676	1.00	65.08	В
MOTA	2989	OH	TYR	В	186	44.420	14.252	29.404	1.00	69.08	В
ATOM	2990	C	TYR	В	186	39.440	10.912	27.513	1.00	50.49	В
MOTA	2991	0	TYR	В	186	39.945	10.682	28.611	1.00	45.48	В
ATOM	2992	N	CYS	В	187	39.430	10.049	26.504	1.00	54.17	В
ATOM	2993	CA	CYS	В	187	40.071	8.745	26.580	1.00	54.62	В
MOTA	2994	C	CYS	В	187	40.984	8.527	25.375	1.00	54.54	В
ATOM	2995	0	CYS	В	187	40.560	8.708	24.235	1.00	53.13	В
ATOM	2996	CB	CYS	В	187	39.027	7.632	26.571		52.62	В
ATOM -	2997	SG	CYS	В	187	37.670	7.762	27.771		59.10	В
ATOM	2998	N			188	42.223	8.110	25.626		54.69	В
ATOM	2999	CA	ALA			43.167	7.838	24.545		49.13	В
ATOM	3000	СВ	ALA			44.470	7.327	25.119		45.83	В
ATOM	3001	C	ALA			42.550	6.804	23.597		46.77	В
ATOM	3002	ō	ALA			42.814	6.807	22.397		50.39	B
ATOM	3003	'N			189	41.718	5.930	24.146		43.31	В
ATOM	3004	CA	LYS			41.036	4.914	23.364		46.05	В
ATOM	3005	CB			189	41.491	3.510	23.770		50.03	В
ATOM	3006	CG	LYS		189	42.999	3.271	23.742		52.69	В
ATOM	3007	CD			189	43.549	3.370	22.335		57.46	В
ATOM	3008	CE			189	42.898	2.356	21.393		54.01	В
ATOM	3009	NZ			189	43.295	2.618	19.969		53.51	В
ATOM	3010	C			189	39.554	5.053	23.682		49.47	В
ATOM	3011	0	LYS		189	39.163	4.994	24.852		52.75	
ATOM	3011	Ŋ			190		5.243	22.661		48.58	В
ATOM	3012	CA			190	38.725 37.296	5.378	22.896		49.55	В
		-									В
ATOM	3014	CB			190	36.535	5.477	21.582		50.32	В
MOTA	3015	OG			190	35.283	4.812	21.694		54.81	В
MOTA	3016	C			190	36.740	4.208	23.693		49.68	В
MOTA	3017	0			190	37.141	3.061	23.500		49.83	В
ATOM	3018	N			191	35.799	4.514	24.583		51.29	В
ATOM	3019	CA			191	35.154	3.504	25.425		46.32	В
ATOM	3020	CB			191	36.149	2.974	26.447		41.82	В
MOTA	3021	CG			191	36.807	4.054	27.266		45.33	В
MOTA	3022	CD			191	37.821	3.492	28.225		47.37	В
MOTA '	3023		GLN			37.474	2.729	29.123		52.60	В
MOTA	3024		GLN			39.086	3.857	28.040		48.36	В
MOTA	3025	C	GLN	В	191	33.939	4.075	26.147	1.00	42.53	В

MOTA	3026	0	GLN	В	191	33.827	5.284	26.340	1.00	39.92	В
ATOM	3027	\mathbf{N} .	ASN	В	192	33.028	3.200	26.546	1.00	44.09	В
ATOM	3028	CA	ASN			31.841	3.648	27.250		45.19	В
ATOM	3029	CB	ASN			30.755	2.607	27.120		45.99	В
ATOM	3030	CG	ASN			30.521	2.221	25.699		57.85	В
ATOM	3031		ASN			30.472	3.084	24.809		62.51	В
ATOM	3032		ASN			30.368	0.920				
ATOM										65.53	В
	3033	C	ASN			32.090	3.947	28.722		45.30	В
ATOM	3034	0	ASN			32.642	3.135	29.469		50.43	В
MOTA	3035	N	LEU			31.678	5.133	29.133		42.79	В
MOTA	3036	CA	LEU			31.828	5.554	30.507		37.15	В
MOTA	3037	CB	LEU			32.700	6.805	30.601	1.00	34.69	В
MOTA	3038	CG	LEU			34.206	6.672	30.424	1.00	37.96	В
ATOM	3039	CD1	LEU	В	193	34.861	8.018	30.702	1.00	30.55	В
MOTA	3040	CD2	LEU	В	193	34.749	5.602	31.375	1.00	40.54	В
ATOM	3041	C	LEU	В	193	30.471	5.876	31.083	1.00	37.77	В
MOTA	3042	0	LEU	В	193	29.516	6.150	30.367	1.00	36.61	В
MOTA	3043	N	GLY	В	194	30.406	5.845	32.401	1.00	40.46	В
MOTA	3044	CA	GLY	В	194	29.187	6.165	33.102	1.00	37.77	В
ATOM	3045	C	GLY			29.683	6.755	34.391		35.59	В
ATOM	3046	0	GLY			30.837	6.516	34.753		34.65	В
ATOM	3047	N	TYR			28.864	7.553	35.065		34.29	В
ATOM	3048	CA	TYR			29.291	8.099	36.345		30.40	В
ATOM	3049	СВ	TYR			29.973	9.447	36.171		27.44	В
ATOM	3050	CG	TYR			29.028	10.573	35.877		40.60	В
ATOM	3051		TYR			28.508	10.758	34.594			
ATOM	3052		TYR							39.19	В
						27.627	11.793	34.330		41.44	В
ATOM	3053	CD2				28.638	11.458	36.891		39.17	В
ATOM	3054	CE2				27.752	12.501	36.635		40.82	В
ATOM	3055	CZ	TYR			27.249	12.662	35.352		41.47	В
ATOM	3056	OH	TYR			26.360	13.680	35.089		42.88	В
ATOM	3057	C	TYR			28.142	8.239	37.323	1.00	30.29	В
MOTA	3058	0	TYR			26.965	8.170	36.950	1.00	31.61	В
MOTA	3059	N	TYR	В	196	28.492	8.393	38.593	1.00	30.42	В
ATOM	3060	CA	TYR	В	196	27.499	8.587	39.639	1.00	29.74	В
MOTA	3061	CB	TYR	В	196	26.939	7.257	40.169	1.00	33.47	В
MOTA	3062	CG	TYR	В	196	27.906	6.391	40.936	1.00	29.20	В
ATOM	3063	CD1	TYR	В	196	28.388	6.771	42.189	1.00	30.92	В
MOTA	3064	CE1	TYR	В	196	29.263	5.967	42.892	1.00	25.31	В
MOTA	3065	CD2	TYR	В	196	28.327	5.185	40.411	1.00	27.03	В
MOTA	3066	CE2	TYR	В	196	29.200	4.374	41.100	1.00	34.13	B
MOTA	3067	CZ	TYR	В	196	29.664	4.764	42.339	1.00	32.37	В
MOTA	3068	OH	TYR			30.511	3.919	43.008	1.00	30.94	В.
ATOM	3069	C	TYR	_		28.136	9.372	40.753		26.07	В
ATOM	3070	ō	TYR			29.355	9.327	40.942	-	22.97	B
MOTA	3071	N	LEU			27.293	10.121	41.456		25.71	В
ATOM	3072	CA	LEU			27.710	10.961	42.566		22.19	В
ATOM	3072	CB	LEU			26.854	12.219	42.592		21.83	В
MOTA	3074	CG	LEU				13.042	41.318		23.28	
						26.959					. В
MOTA	3075		LEU			26.111	14.287	41.458		27.40	В
MOTA	3076		LEU			28.415	13.415	41.071		25.75	В
MOTA	3077	C	LEU			27.578	10.200	43.881		19.99	В
MOTA	3078	0	LEU			26.825	9.230	43.995		19.34	В
MOTA	3079	N	SER			28.307	10.661	44.879		18.26	В
MOTA	3080	CA	SER			28.314	10.010	46.175	1.00	19.64	В
MOTA	3081	CB	SER			29.369	8.911	46.173		20.93	В
MOTA	3082	OG	SER			30.661	9.507	46.033	1.00	23.70	В
ATOM	3083	C	SER	В	198	28.666	11.027	47.252	1.00	21.67	В

MOTA	3084	0	SER	В	198	29	.533	11.884	47.065	1.00	15.06	В
MOTA	3085	N	GLY	В	199	28	.005	10.901	48.394	1.00	24.20	В
MOTA	3086	CA	GLY	В	199	28	.252	11.815	49.485	1.00	22.78	В
MOTA	3087	C	GLY	В	199		.063	11.890	50.411	1.00	24.70	В
MOTA	3088	0	GLY			26	.008	11.329	50,128	1.00	26.26	В
ATOM	3089	N	THR	В	200	27	.239	12.585	51.526	1.00	28.78	В
MOTA	3090	CA	THR			26	.183	12.741	52.517	1.00	31.30	В
MOTA	3091	CB	THR	В	200	26	.724	13.391	53.773	1.00	30.61	В
ATOM	3092	OG1	THR	\mathbf{B}	200	27	.818	12.620	54.248	1.00	29.07	В
MOTA	3093	CG2					.666	13.435	54.843	1.00	37.01	В
ATOM	3094	C	THR	В	200	25	.057	13.593	51.973	1.00	28.61	В
MOTA	3095	0	THR	В	200	25	.282	14.688	51.477	1.00	27.34	В
ATOM	3096	N	THR	В	201	23	.841	13.085	52.090	1.00	28.10	В
MOTA	3097	CA	THR			22	.675	13.765	51.560	1.00	30.23	В
ATOM	3098	CB	THR			21	.937	12.796	50.633	1.00	26.26	В
ATOM	3099	OG1	THR	В	201	22	.347	13.056	49.289	1.00	30.41	В
MOTA	3100	CG2	THR	В	201	20	.437	12.920	50`.781	1.00	34.96	В
MOTA	3101	С	THR				.746	14.314	52.634	1.00	30.10	В
ATOM	3102	0	THR			21	.719	13.806	53.754	1.00	32.16	В
ATOM	3103	N	ALA			20	.963	15.333	52.294	1.00	26.57	В
ATOM	3104	CA	ALA			20	.082	15.919	53.293	1.00	26.82	В
MOTA	3105	CB	ALA			20	.438	17.397	53.492	1.00	17.25	В
ATOM	3106	С	ALA			18	.606	15.795	52.992	1.00	26.52	В
ATOM	3107	0	ALA				.791	16.392	53.691		28.78	В
ATOM	3108	N	ASP				.248	15.018	51.977	1.00	26.44	В
ATOM	3109	CA	ASP				.839	14.906	51.593		23.32	В
ATOM	3110	CB	ASP				.564	15.802	50.400		25.97	В
ATOM	3111	CG	ASP				.479	15.509	49.226		32.36	В
ATOM	3112		ASP				.976	15.347	48.096		39.58	В
MOTA	3113		ASP				.706	15.443	49.424		38.65	В
ATOM	3114	C	ASP				.423	13.507	51.239		25.20	В
ATOM	3115	0	ASP				.264	12.666	50.946		31.85	В
ATOM	3116	N	ALA				.120	13.257	51.268		23.17	В
ATOM	3117	CA	ALA				.574	11.947	50.948		22.41	В
MOTA	3118	CB	ALA				.111	11.927	51.227		13.89	В
ATOM	3119	C	ALA				.829	11.585	49.483		29.93	В
ATOM	3120	0	ALA				.913	10.405	49.132		36.73	В
MOTA	3121	N	GLY				.950	12.595	48.628		28.61	В
ATOM	3122	CA	GLY				.214	12.334	47.226		31.44	В
MOTA	3123	C	GLY				.695	12.060	47.041		31.13	В
ATOM	3124	0	GLY				.185	11.808	45.941		29.42	В
ATOM ATOM	3125 3126	N CA	ASN				.414	12.136	48.147		33.30	В
ATOM	3127	CB	ASN ASN				.838 .057	11.868	48.161		35.99	В
ATOM	3127							10.351	48.046		34.91	В
ATOM	3129	CG	ASN ASN				.506 .069	9.950 9.219	48.241		40.27	В
ATOM	3130						.118		47.428		46.66	В
ATOM	3131	C	ASN					10.424	49.322 47.088		39.62	В
ATOM	3132	0	ASN ASN				.639 .594	12.617 12.078	46.537		34.31 32.67	В
ATOM	3133	N	SER				.282	13.868	46.814		35.04	В
ATOM	3134	CA	SER				.013	14.619	45.795		34.71	В
ATOM	3135	CB	SER				.179	14.732	44.527		35.48	В
ATOM	3136	OG	SER				.189	15.717				В
ATOM	3137	C	SER				. 483	16.014	44.697 46.188		39.62 29.99	В
ATOM	3138	0	SER				.903	16.778	45.331		33.75	В
ATOM	3139	N	ILE				.402	16.778	47.469		33.75 27.75	В
ATOM	3140	CA	ILE				.856	17.658	47.469			В
MOTA	3141	CB	ILE				.725	18.408	48.684		26.41	B B
OI-1			تالات	_	~00		. 125	TO.409	40.004	. 1.00	エフ・サン	Þ

ATOM	3142	CG2	ILE B	208	20.202	19.751	49.125	1.00 15.89	В
MOTA	3143	CG1	ILE B	208	18.545	18.582	47.727	1.00 22.27	В
MOTA	3144	CD1	ILE B	208	17.268	18.938	48.379	1.00 24.92	Ė
ATOM	3145	C	ILE B	208	21.991	17.380	48.938	1.00 31.88	В
ATOM	3146	0	ILE B	208	21.776	16.879	50.046	1.00 35.04	В
ATOM	3147	N	PHE B		23.208	17.687	48.514	1.00 36.15	В
ATOM	3148	CA	PHE B		24.360	17.400	49.344	1.00 39.16	В
MOTA	3149	CB	PHE B		25.629	17.332	48.483	1.00 36.39	В
ATOM	3150	CG	PHE B		25.646	16.150	47.549	1.00 33.22	В
ATOM	3151		PHE B		25.014	16.218	46.304	1.00 30.15	В
MOTA	3152		PHE B		26.193	14.933	47.962	1.00 30.13	В
ATOM	3153		PHE B		24.914	15.089	45.481	1.00 31.74	
ATOM	3154	CE2	PHE B		26.101	13.793	47.151	1.00 37.20	В
ATOM	3155	CZ	PHE B		25.455	13.873		1.00 37.20	B B
ATOM	3156	C.	PHE B		24.541	18.317	50.523	1.00 34.03	
ATOM	3157	ō	PHE B		24.651	19.530	50.383		В
ATOM	3158	N	THR B		24.542	17.691		1.00 47.02	В
ATOM	3159	CA	THR B		24.542		51.693	1.00 46.95	В
ATOM	3160	CB	THR B		25.045	18.335	52.991	1.00 49.81	В
ATOM		OG1				17.276	54.045	1.00 50.33	В
MOTA	3161	CG2	THR B		23.877	16.496	54.329	1.00 52.23	В
	3162 3163				25.582	17.916	55.309	1.00 52.39	В
MOTA		C	THR B		25.752	19.424	53.039	1.00 52.19	В
MOTA	3164	0	THR B		26.828	19.282	52.459	1.00 49.93	В
MOTA	3165	N	ASN B		25.437	20.508	53.747	1.00 56.58	В
MOTA	3166	CA	ASN B		26.376	21.610	53.884	1.00 58.40	В
ATOM	3167	CB	ASN B		25.683	22.880	54.368	1.00 60.22	В
ATOM	3168	CG	ASN B		26.656	24.041	54.537	1.00 62.16	В
MOTA	3169		ASN B		26.264	25.136	54.933	1.00 67.38	. B
MOTA	3170		ASN B		27.928	23.804	54.232	1.00 57.41	В
ATOM	3171	C	ASN B		27.459	21.242	54.872	1.00 58.42	В
MOTA	3172	0	ASN B		27.198	21.008	56.048	1.00 57.03	В
ATOM	3173	N	THR B		28.683	21.202	54.376	1.00 60.52	В
MOTA	3174	CA	THR B		29.831	20.864	55.191	1.00 64.62	В
MOTA	3175	CB	THR B		30.573	19.674	54.577	1.00 61.43	В
ATOM	3176	OG1	THR B		29.848	18.474	54.862	1.00 55.72	B
ATOM	3177	CG2	THR B		31.987	19.578	55.118	1.00 62.96	В
ATOM	3178	C	THR B		30.765	22.065	55.276	1.00 70.20	В
MOTA	3179	0	THR B		31.455	22.395	54.312	1.00 71.19	В
ATOM	3180	N	ALA B		30.780	22.716	56.432	1.00 73.39	В
MOTA	3181	CA	ALA B		31.623	23.882	56.636	1.00 76.16	В
ATOM	3182	CB	ALA B		31.195	25.004	55.696	1.00 69.82	В
ATOM	3183	C	ALA B		31.504	24.334	58.081	1.00 78.85	В
MOTA	3184	0	ALA B		30.491	24.073	58.739	1.00 74.22	В
ATOM	3185	N	SER B		32.537	25.014	58.572	1.00 85.01	В
MOTA	3186	CA	SER B		32.520	25.499	59.943	1.00 90.59	· B
MOTA	3187	CB	SER B		33.896	25.327	60.584	1.00 89.01	В
MOTA	3188	OG	SER B		33.814	25.478	61.993	1.00 90.44	. В
MOTA	3189	C	SER B		32.074	26.965	60.048	1.00 94.26	В
ATOM	3190	0	SER B		31.036	27.249	60.652	1.00 92.95	В
ATOM	3191	N	PHE B		32.839	27.884	59.454	1.00 97.92	В
MOTA	3192	CA	PHE B		32.507	29.316	59.510	1.00102.65	В
MOTA	3193	CB	PHE B		33.226	30.099	58.403	1.00110.99	В
MOTA	3194	CG	PHE B		32.937	31.591	58.424	1.00120.75	В
MOTA	3195		PHE B		32.974	32.342	57.247	1.00124.12	В
MOTA	3196		PHE B		32.626	32.244	59.621	1.00122.39	В
ATOM	3197	CE1	PHE B	215	32.705	33.716	57.259	1.00124.99	В
MOTA	3198	CE2		215	32.357	33.614	59.644	1.00124.51	• в
MOTA	3199	CZ	PHE B	215	32.396	34.352	58.461	1.00125.83	В

MOTA	3200	C	PHE	В	215	31.008	29.612	59.417	1.00101.78	. В
ATOM	3201	0	PHE	В	215	30.452	29.729	58.320	1.00 98.40	В
MOTA	3202	N	SER	В	216	30.378	29.766	60.580	1.00102.30	В
MOTA	3203	CA	SER	В	216	28.950	30.043	60.669	1.00102.31	В
MOTA	3204	CB	SER	₿	216 ·	28.690	31.550	60.635	1.00104.47	В
MOTA	3205	OG	SER	В	216	27.323	31.825	60.897	1.00107.31	В
MOTA	3206	C	SER	В	216	28.237	29.360	59.511	1.00100.63	В
ATOM	3207	0	SER		216	28.033	29.949	58.446	1.00102.98	В
MOTA	3208	N	PRO			27.848	28.099	59.711	1.00 96.87	В
ATOM	3209	CD	PRO	В	217	27.869	27.384	60.999	1.00 96.34	В
MOTA	3210	CA	PRO			27.158	27.307	58.694	1.00 93.40	В
MOTA	3211	CB	PRO			26.965	25.964	59.384	1.00 94.81	В
MOTA	3212	CG	PRO			26.768	26.368	60.811	1.00 96.22	В
MOTA	3213	C	PRO			25.840	27.892	58.219	1.00 88.20	В
MOTA	3214	0	PRO			24.821	27.745	58.889	1.00 86.80	В
ATOM	3215	N	ALA			25.864	28.559	57.069	1.00 81.43	В
MOTA	3216	CA	ALA			24.644	29.111	56.517	1.00 77.92	B
ATOM	3217	CB	ALA			24.885	29.605	55.108	1.00 74.00	. В
ATOM	3218	C	ALA			23.671	27.939	56.503	1.00 76.24	В
ATOM	3219	0	ALA			23.587	27.206	55.520	1.00 81.49	В
ATOM	3220	N	GLN			22.944	27.760	57.597	1.00 71.04	В
ATOM	3221	CA	GLN			22.006	26.654	57.718	1.00 70.90	В
ATOM	3222	CB	GLN			21.485	26.572	59.146	1.00 73.31	В
ATOM	3223	CG	GLN			20.490	25.451	59.348	1.00 80.97	В
ATOM	3224	CD	GLN			19.824	25.516	60.695	1.00 86.76	В
ATOM	3225		GLN		219	18.982	24.679	61.027	1.00 92.84	В
ATOM	3226	NE2				20.193	26.519	61.486	1.00 90.33	В
MOTA	3227	C	GLN			20.806	26.691	56.781	1.00 68.73	В
ATOM	3228	0	GLN			20.396	27.755	56.326	1.00 68.60	В
MOTA	3229	N	GLY			20.253	25.513	56.497	1.00 66.84	В
MOTA	3230	CA	GLY			19.066	25.422	55.658	1.00 65.64	В
ATOM ATOM	3231	C	GLY			19.200	25.250	54.156	1.00 62.93	В
ATOM	3232 3233	N O	GLY VAL			18.197 20.419	25.016	53.474	1.00 60.58	. B
MOTA	3234	CA	VAL			20.419	25.350 25.209	53.634 52.206	1.00 59.50	В
ATOM	3235	CB	VAL			21.492	26.346	51.648	1.00 56.77	В
ATOM	3236	CGI				21.306	26.455	50.145	1.00 56.11	В
ATOM	3237		VAL			21.128	27.644	52.300	1.00 52.54	B B
MOTA	3238	C	VAL			21.120	23.853	51.789	1.00 56.04	В
ATOM	3239	Ö	VAL			20.626	22.816	52.117	1.00 55.23	B
ATOM	3240	N	GLY			22.308	23.863	51.066	1.00 54.20	В
ATOM	3241	CA	GLY			22.895	22.625	50.584	1.00 49.22	В
MOTA	3242	C	GLY			23.086	22.689	49.076	1.00 44.37	B
MOTA	3243	ō	GLY			22.327	23.351	48.384	1.00 45.67	В
ATOM	3244	N	VAL			24.099	21.995	48.571	1.00 39.98	В
MOTA	3245	CA	VAL			24.433	21.976		1.00 34.73	В
MOTA	3246	CB	VAL	В	223	25.960	21.887	46.972	1.00 37.08	В
MOTA	3247		VAL			26.316	21.712	45.508	1.00 37.73	В
ATOM	3248		VAL			26.621	23.129	47.564	1.00 33.20	В
ATOM	3249	C	VAL	В	223	23.799	20.825	46.354	1.00 34.60	В
ATOM	3250	0	VAL	В	223	23.819	19.671	46.790	1.00 35.57	В
MOTA	3251	N	GLN	В	224	23.236	21.141	45.188	1.00 32.64	В
ATOM	3252	CA	GLN	В	224	22.611	20.125	44.334	1.00 31.49	В
MOTA	3253	CB	GLN	В	224	21.103	20.311	44.282	1.00 20.31	В
MOTA	3254	CG	GLN			20.376	19.195	43.586	1.00 27.39	В
MOTA	3255	CD	GLN			18.894	19.490	43.414	1.00 32.58	В
MOTA	3256		GLN			18.052	18.609	43.538	1.00 38.46	В
MOTA	3257	NE2	GLN	В	224	18.573	20.739	43.118	1.00 37.37	В

MOTA	3258	C	GLN	В	224	23.204	20.270	42.933	1.00 34	.63	В
MOTA	3259	0	GLN	В	224	23.372	21.384	42.439	1.00 35	.45	В
MOTA	3260	N	LEU	В	225	23.558	19.152	42.306	1.00 32	. 63	В
MOTA	3261	CA	LEU	В	225	24.152	19.212	40.988	1.00 26	.59	В
MOTA	3262	CB	LEU	В	225	25.362	18.295	40.897	1.00 26	.01	В
ATOM	3263	CG	LEU		225	26.470	18.573	41.909	1.00 28	.03	В
MOTA	3264	CD1	LEU	В	225	27.738	17.835	41.509	1.00 28	.60	В
ATOM	3265	CD2	LEU	В	225	26.739	20.045	41.970	1.00 29	. 82	В
MOTA	3266	C	LEU	В	225	23.152	18.860	39.921	1.00 29	.18	В
MOTA	3267	0	LEU	В	225	22.297	17.972	40.082	1.00 30	. 83	В
ATOM	3268	N	THR	В	226	23.284	19.556	38.804	1.00 26	.74	В
ATOM	3269	CA	THR			22.369	19.358	37.714	1.00 26	.34	В
MOTA	3270	CB	THR			21.411	20.570	37.722	1.00 23	.75	В
ATOM	3271	OG1				20.156	20.204	37.154	1.00 31	.98	В
ATOM	3272	CG2	THR	В	226	22.018	21.731	36.989	1.00 24	.18	В
ATOM	3273	C	THR			23.157	19.202	36.398	1.00 25	.37	В
MOTA	3274	0	THR			24.279	19.712	36.272	1.00 22.	. 87	В
MOTA	3275	N	ARG			22.599	18.450	35.451	1.00 25.	.59	В
MOTA	3276	CA	ARG			23.239	18.232	34.142	1.00 28.	. 66	В
MOTA	3277	CB	ARG			23.658	16.742	33.950	1.00 24	.62	В
MOTA	3278	CG	ARG	_		22.522	15.718	34.034	1.00 21.	.48	В
MOTA	3279	CD	ARG			23.019	14.269	33.901	1.00 32.	.32	В
ATOM	3280	NE	ARG			22.016	13.390	33.284	1.00 29.		В
ATOM	3281	CZ	ARG			21.197	12.582	33.947	1.00 34.		B
MOTA	3282		ARG			21.248	12.513	35.277	1.00 41.		В
ATOM	3283		ARG			20.309	11.854	33.278	1.00 32.		В
ATOM	3284	C	ARG			22.229	18.683	33.079	1.00 31.		В
ATOM	3285	0	ARG			21.265	17.967	32.747	1.00 26.		В
ATOM	3286	N	ASN			22.462	19.890	32.561	1.00 38.		В
MOTA	3287	CA	ASN			21.559	20.508	31.589	1.00 41.		В
ATOM	3288	CB	ASN			21.654	19.805	30.234	1.00 48.		B
ATOM	3289	CG	ASN			22.927	20.151	29.497	1.00 57.		В
ATOM	3290		ASN			23.022	19.949	28.288	1.00 65.		В
ATOM	3291		ASN			23.919	20.675	30.222	1.00 55.		В
MOTA MOTA	3292	C	ASN ASN			20.118	20.469	32.108	1.00 39.		В
	3293	0				19.196	20.002	31.430	1.00 36.		В
MOTA MOTA	3294	N CA	GLY GLY			19.934	20.930	33.337	1.00 38.		В
MOTA	3295 3296	CA	GLY			18.605	20.950	33.908	1.00 41.		В
ATOM	3290	o	GLY			18.155 17.287	19.725 19.843	34.678 35.549	1.00 43.		B B
ATOM	3298	N	THR			18.711	18.557	34.364	1.00 43.		В
MOTA	3299	CA.	THR			18.332	17.333	35.056	1.00 38.		В
ATOM	3300	CB	THR			18.610	16.113	34.211	1.00 30.		В
ATOM	3301	OG1	THR			17.7.06	16.096	33.109	1.00 40.		В
MOTA	3302	CG2	THR			18.431	14.841	35.036	1.00 38.		. B
ATOM	3303	C	THR			19.100	17.179	36.351	1.00 39.		В
ATOM	3304	ō	THR			20.323	17.354	36.391	1.00 42.		. В
ATOM	3305	N	ILE			18.372	16.847	37.409	1.00 34.		В
MOTA	3306	CA	ILE			18.968	16.670	38.720	1.00 30.		В
MOTA	3307	CB	ILE			17.889.	16.703	39.830	1.00 35.		В
ATOM	3308	CG2	ILE	В	231	18.467	16.211	41.162	1.00 31.		В
MOTA	3309		ILE	В	231	17.337	18.118	39.979	1.00 31.		В
ATOM	3310		ILE			16.245	18.219	41.030	1.00 38.		В
ATOM	3311	C	ILE			19.690	15.346	38.784	1.00 28.		В
MOTA	3312	0	ILE			19.227	14.345	38.238	1.00 28.		В
MOTA	3313	N	ILE			20.829	15.341	39.460	1.00 28.		В
ATOM	3314	CA	ILE			21.605	14.119	39.598	1.00 26.		В
MOTA	3315	CB	ILE	В	232	23.052	14.347	39.122	1.00 26.		В

MOTA	3316	CG2	ILE	в :	232	23.856	13.055	39.214	1.00	23.10	В
MOTA	3317		ILE			23.048	14.846	37.670	1.00	27.40	В
MOTA	3318	CD1	ILE			24.387	15.385	37.201	1.00	14.12	В
ATOM	3319	C	ILE	В :	232	21.624	13.648	41.053	1.00	29.16	В
MOTA	3320	0	ILE :	В :	232	22.390	14.157	41.877	1.00	33.06	·B
ATOM	3321	N	PRO :	В :	233	20.744	12.703	41.406	1.00	26.93	В
MOTA	3322	CD	PRO :			19.503	12.296	40.730	1.00	17.70	В
MOTA	3323	CA	PRO :			20.771	12.239	42.800	1.00	27.35	В
ATOM	3324	CB	PRO :	В :	233	19.422	11.522	42.959	1.00	25.87	В
MOTA	3325	CG	PRO :	в :	233	19.057	11.133	41.563	1.00	24.73	В
MOTA	3326	С	PRO :	В :	233	21.967	11.306	42.996	1.00	27.88	В
MOTA	3327	0	PRO :	в :	233	22.426	10.676	42.043	1.00	31.92	В
ATOM	3328	N	ALA :			22.476	11.237	44.218	1.00	26.36	В
MOTA	3329	CA	ALA :	в :	234	23.617	10.383	44.547	1.00	23.38	В
MOTA	3330	CB	ALA :	в :	234	23.908	10.470	46.019	1.00	21.51	В
MOTA	3331	C	ALA :	в :	234	23.358	8.938	44.178	1.00	23.04	В
MOTA	3332	0	ALA :	B :	234	22.255	8.442	44.379	1.00	22.78	В
MOTA	3333	N	ASN :			24.375	8.267	43.635	1.00	21.90	В
MOTA	3334	CA	ASN :			24.260	6.859	43.259	1.00	24.10	В
ATOM .	3335	CB	ASN :	В 2	235	23.996	6.020	44.508	1.00	22.91	В
ATOM	3336	CG	ASN :			25.033	6.275	45.585	1.00	33.34	В
MOTA	3337		ASN :			24.726	6.808	46.655		35.54	В
MOTA	3338		ASN :			26.278	5.921	45.296	1.00	26.96	В
MOTA	3339	C	ASN !			23.220	6.539	42.191		27.36	В
MOTA	3340	0	ASN :			22.502	5.541	42.285		29.41	В
MOTA	3341	N	ASN I			23.149	7.402	41.182		28.35	В
ATOM	3342	CA	ASN I			22.250	7.252	40.048		28.60	В
ATOM	3343	CB	ASN I			21.262	8.425	40.002		40.03	В
ATOM	3344	CG	ASN I			20.472	8.490	38.694		41.42	В
ATOM	3345		ASN I			19.769	7.556	38.342		47.61	В
ATOM	3346		ASN :			20.593	9.602	37.975		50.59	· В
ATOM	3347	C	ASN 1			23.220	7.311	38.873		31.22	В
ATOM	3348	0	ASN 1			23.697	8.383	38.521		35.01	В
ATOM	3349	N	THR I			23.529	6.172	38.270		27.12	В
ATOM	3350	CA	THR I			24.497	6.180	37.195		31.43	В
ATOM	3351	CB	THR I			24.953	4.733	36.841		38.77	В
ATOM	3352		THR I			25.264	4.009	38.045		43.58	В
MOTA	3353	CG2	THR I			26.203	4.778	35.974		38.34	В
ATOM ATOM	3354 3355	C	THR I			24.056 23.035	6.899 6.578	35.929 35.326		30.75	В
ATOM	3356	N	VAL I			24.842	7.888	35.536		31.22	B B
ATOM	3357	CA	VAL :			24.562	8.642	34.330		36.89	В
ATOM	3358	CB	VAL			24.856	10.144	34.504		42.58	В
ATOM	3359		VAL			24.820	10.845	33.145		38.47	В
ATOM	3360		VAL			23.830	10.764	35.427		49.26	В
ATOM	3361	C	VAL I			25.473	8.108	33.243			
MOTA	3362	ŏ	VAL			26.703	8.139	33.370		36.75	В
ATOM	3363	N	SER			24.861	7.628	32.171		40.84	В
ATOM	3364	CA	SER			25.617	7.078	31.067		41.99	В
ATOM	3365	CB	SER			24.780	6.074	30.311		43.25	В
MOTA	3366	OG	SER I			25.514	5.637	29.189		55.86	В
MOTA	3367	C	SER			26.109	8.117	30.085		40.52	В
ATOM	3368	0	SER			25.321	8.789	29.435		44.65	B
MOTA	3369	N	LEU !			27.421	.8.223	29.965		38.57	В
MOTA	3370	CA	LEU :			28.047	9.171	29.054		36.39	В
ATOM	3371	CB	LEU I			29.435	9.509	29.557		27.79	В
MOTA	3372	CG	LEU I			29.508	10.513	30.690		29.69	В
MOTA	3373	CD1	LEU 1	в 2	240	30.942	10.583	31.194		30.85	В

MOTA	3374	CD2	LEU E	3 240	29.032	11.874	30.202	1.00 21.59	В
ATOM	3375	C	LEU E	3 240	28.168	8.673	27.610	1.00 38.07	В
MOTA	3376	0	LEU E	3 240	28.503	9.450	26.722	1.00 34.28	В
ATOM	3377	N	GLY I		27.900	7.388	27.380	1.00 41.68	В
ATOM	3378	CA	GLY E		28.026	6.836	26.041	1.00 43.13	В
ATOM	3379	C	GLY E		29.493	6.588	25.717	1.00 45.49	В
ATOM	3380	Õ	GLY I		30.274	6.251	26.603	1.00 47.59	В
ATOM		N	ALA E			6.754			
	3381				29.882		24.457	1.00 44.97	В
ATOM	3382	CA	ALA I		31.272	6.549	24.078	1.00 43.27	В
ATOM	3383	CB	ALA E		31.369	6.048	22.666	1.00 43.85	В
MOTA	3384	C	ALA E		32.029	7.847	24.203	1.00 43.58	В
MOTA	3385	0	ALA E		31.602	8.877	23.694	1.00 46.79	В
ATOM	3386	N	VAL E		33.154	7.791	24.899	1.00 43.90	В
MOTA	3387	CA	VAL E	3 243	33.995	8.956	25.088	1.00 45.15	В
ATOM	3388	CB	VAL E	3 243	213,34	9.237	26.561	1.00 41.04	В
MOTA	3389	CG1	VAL E	3 243	35.072	10.480	26.729	1.00 42.50	В
ATOM	3390	CG2	VAL E	243	32.882	9.414	27.232	1.00 46.97	В
MOTA	3391	С	VAL E	243	35.338	8.649	24.442	1.00 49.51	В
ATOM	3392	0	VAL E	243	35.942	7.606	24.719	1.00 53.18	В
ATOM	3393	N	GLY E	244	35.797	9.557	23.587	1.00 46.10	В
MOTA	3394	CA	GLY E		37.046		22.903	1.00 45.94	В
ATOM	3395	C	GLY E		38.098	10.409	23.107	1.00 49.17	В
ATOM	3396	ō	GLY E		38.265	10.946	24.209	1.00 49.15	В
ATOM	3397	N	THR E		38.809	10.716	22.024	1.00 51.75	В
ATOM	3398	CA	THR E		39.898	11.685	22.055	1.00 51.75	В
		CB	THR E		40.769				
ATOM	3399					11.560	20.776	1.00 50.87	В
ATOM	3400.	OG1			39.935	11.583	19.610	1.00 54.40	В
ATOM	3401	CG2	THR E		41.532	10.245	20.795	1.00 43.64	В
ATOM	3402	C	THR E		39.442	13.115	22.264	1.00 51.21	В
ATOM	3403	0	THR E		40.195	13.940	22.781	1.00 53.72	В
ATOM	3404	N	SER E		38.206	13.406	21.871	1.00 52.18	В
MOTA	3405	CA	SER E		37.649	14.743	22.059	1.00 52.11	В
MOTA	3406	CB	SER E		36.619	15.067	20.977	1.00 53.99	В
ATOM	3407	OG	SER E	246	37.102	14.741	19.688	1.00 64.44	В
MOTA	3408	C	SER E	246	36.952	14.726	23.414	1.00 49.45	В
MOTA	3409	0	SER E	246	36.090	13.880	23.659	1.00 48.06	В
MOTA	3410	N	ALA E	247	37.337	15.651	24.287	1.00 47.65	В
ATOM	3411	CA	ALA E	247	36.747	15.759	25.614	1.00 47.77	В
ATOM	3412	CB	ALA E	247	37.324	16.959	26.333	1.00 47.73	В
ATOM	3413	C	ALA E	247	35.221	15.873	25.569	1.00 48.47	В
ATOM	3414	0	ALA E		34.641	16.428	24.639	1.00 50.29	В
MOTA	3415	N	VAL E	248	34.575	15.330	26.585	1.00 46.82	В
ATOM	3416	CA	VAL E		33.133	15.383	26.681	1.00 46.36	В
MOTA	3417	CB	VAL E		32.516	13.981	26.698	1.00 46.49	В
ATOM	3418		VAL E		31.044	14.066	27.053	1.00 44.07	В
ATOM	3419		VAL E		32.701	13.319	25.349	1.00 46.22	В
ATOM	3420	C	VAL E		32.803	16.074	27.988	1.00 49.23	. В
MOTA	3421		VAL E		33.256	15.656	29.057	1.00 49.23	. В
		0			32.018				
MOTA	3422	N	SER E			17.138	27.893	1.00 48.19	В
ATOM	3423	CA	SER E		31.609	17.903	29.060	1.00 46.49	В
MOTA	3424	CB	SER E		31.191	19.308	28.626	1.00 44.33	В
ATOM	3425	OG	SER E		30.934	20.145	29.733	1.00 42.86	В
ATOM	3426	C	SER E		30.430	17.193	29.703	1.00 45.02	В
MOTA	3427	0	SER E		29.502	16.800	29.003	1.00 42.57	В
MOTA	3428	N	LEU E		30.463	17.006	31.022	1.00 45.38	В
MOTA	3429	CA	LEU E		29.336	16.354	31.700	1.00 46.18	В
ATOM	3430	CB	LEU E		29.716	15.920	33.121	1.00 47.35	В
MOTA	3431	CG	LEU E	3 250	30.926	14.995	33.318	1.00 50.12	В

MOTA	3432		LEU E		30.880	14.434	34.742	1.00 42.80	В
MOTA	3433	CD2	LEU E		30.915	13.859	32.294	1.00 47.40	В
MOTA	3434	C	LEU E	250	28.164	17.340	31.765	1.00 44.55	В
ATOM	3435	0	LEU E	250	27.020	16.954	32.031	1.00 40.92	В
MOTA	3436	N	GLY E	251	28.468	18.613	31.512	1.00 38.11	В
MOTA	3437	CA	GLY E	251	27.451	19.640	31.545	1.00 39.35	В
ATOM -	3438	С	GLY F	251	26.857	19.780	32.930	1.00 38.25	В
MOTA	3439	0	GLY E	251	25.637	19.768	33.106	1.00 42.31	В
MOTA	3440	N	LEU E	252	27.733	19.922	33.911	1.00 34.29	В
ATOM	3441	CA	LEU E	252	27.326	20.043	35.294	1.00 36.24	В
MOTA	3442	CB	LEU E	252	28.352	19.364	36.206	1.00 32.99	В
MOTA	3443	CG	LEU E		28.547	17.852	36.082	1.00 30.21	В
MOTA	3444		LEU E		29.689	17.451	36.982	1.00 24.12	В
MOTA	3445	CD2	LEU E	252	27.276	17.110	36.449	1.00 27.28	В
ATOM	3446	C	LEU E		27.169	21.480	35.757	1.00 39.41	В
MOTA	3447	ŏ .	LEU E		27.865	22.375	35.294	1.00 43.64	В
ATOM	3448	N	THR E		26.243	21.688	36.682	1.00 38.02	В
ATOM	3449	CA	THR E		26.016	22.996	37.271	1.00 37.82	В
ATOM	3450	CB	THR E		24.796	23.700	36.677	1.00 40.67	В
ATOM	3451	OG1	THR E		25.162	24.342	35.450	1.00 47.87	В
ATOM	3452	CG2			24.254	24.724	37.659	1.00 27.23	В
ATOM	3453	C	THR E		25.729	22.771	38.736	1.00 39.11	В
ATOM	3454	ō	THR E		24.958	21.868	39.088	1.00 40.91	В
ATOM	3455	N	ALA E		26.361	23.574	39.584	1.00 35.35	В
ATOM	3456	CA	ALA E		26.126	23.492	41.016	1.00 36.35	В
ATOM	3457	СВ	ALA E		27.360	23.962	41.786	1.00 29.54	В
ATOM	3458	C	ALA E		24.922	24.406	41.314	1.00 41.67	В
ATOM	3459	Õ	ALA E		24.836	25.539	40.826	1.00 44.92	В
ATOM	3460	N	ASN B		23.989	23.904		1.00 40.95	В
ATOM	3461	CA	ASN E		22.796	24.660	42.463	1.00 36.68	В
ATOM	3462	CB	ASN E		21.566	24.036	41.819	1.00 30.00	В
ATOM	3463	CG	ASN B		21.675	23.942	40.341	1.00 32.34	В
ATOM	3464		ASN E		21.160	24.783	39.626	1.00 37.84	В
ATOM	3465		ASN E		22.343	22.912	39.862	1.00 40.27	В
MOTA	3466	C	ASN E		22.568	24.596	43.953	1.00 35.83	В
ATOM	3467	ō	ASN E		22.895	23.593	44.585	1.00 40.02	В
ATOM	3468	N	TYR E		22.004	25.654	44.521	1.00 34.15	В
ATOM	3469	CA	TYR E		21.655	25.612	45.933	1.00 30.18	В
ATOM	3470	CB	TYR E		21.647	27.002	46.559	1.00 30.18	В
ATOM	3471	CG	TYR E		22.988	27.687	46.675	1.00 24.00	В
MOTA	3472		TYR E		23.343	28.712	45.795	1.00 26.24	В
ATOM	3473	CE1			24.530	29.427	45.955	1.00 20.24	В
ATOM	3474	CD2	TYR E		23.861	27.379	47.715	1.00 32.40	В
ATOM	3475	CE2	TYR E		25.056	28.081	47.887	1.00 24.37	В
ATOM	3476	CZ	TYR E		25.387	29.108	47.007	1.00 35.56	В
ATOM	3477	OH	TYR E		26.559	29.817	47.178	1.00 33.30	В
ATOM	3478	C	TYR E		20.226	25.042	45.980	1.00 29.03	В
ATOM	3479	Ö	TYR E		19.391	25.350	45.128	1.00 28.10	. B
ATOM	3480	N	ALA E		19.959	24.173	46.941	1.00 28.10	. В
ATOM	3481	CA	ALA E		18.626	23.614	47.112	1.00 31.43	
		CB	ALA E		18.606	22.164	46.739	1.00 35.79	B B
ATOM	3482	C	ALA E						
ATOM	3483		ALA E		18.339	23.781	48.595	1.00 40.06	В
ATOM	3484	O N	ARG E		19.263	23.907	49.405	1.00 37.56	В
MOTA	3485	N	ARG E		17.070	23.805	48.960	1.00 46.77	В
ATOM	3486	CA	ARG E		16.736	23.969	50.367	1.00 53.74	В
MOTA	3487	CB	ARG E		15.509	24.870	50.531	1.00 59.02	В
ATOM	3488	CG			15.714	26.319	50.133	1.00 59.88	В
MOTA	3489	CD	ARG F	458	14.404	27.057	50.243	1.00 69.10	В

MOTA	3490	NE	ARG 1	3 258 ·	13.882	27.004	51.605	1.00 78.61	В
MOTA	3491	cz	ARG I	3 258	12.611	27.224	51.923	1.00 83.09	В
MOTA	3492	NH1	ARG I		11.732	27.506	50.972	1.00 87.22	В
MOTA	3493		ARG I		12.219	27.169	53.190	1.00 84.52	В
MOTA	3494	C		3 258	16.468	22.623	51.009	1.00 55.40	. B
ATOM	3495	ō		3 258	15.737	21.791		1.00 55.46	
ATOM	3496	И		3 259	17.058		50.457		В
						22.430	52.183	1.00 56.01	В
MOTA	3497	CA		3 259	16.915	21.194	52.932	1.00 58.80	В
ATOM	3498	CB		3 259	18.159	20.915	53.753	1.00 60.30	В
ATOM	3499	OG1			18.521	22.094	54.479	1.00 62.86	В
ATOM	3500	CG2	THR I		19.306	20.503	52.853	1.00 65.59	В
ATOM	3501	C		3 259	15.755	21.277	53.887	1.00 62.14	В
ATOM	3502	0	THR I	3 259	14.654	20.827	53.576	1.00 61.18	В
MOTA	3503	И	GLY E	3 260	16.027	21.863	55.054	1.00 68.48	В
ATOM	3504	CA	GLY E	3 260	15.025	22.024	56.094	1.00 69.86	ÌВ
ATOM	3505	С	GLY E	3 260	13.984	23.075	55.777	1.00 70.03	В
ATOM	3506	0	GLY E		13.201	22.915	54.839	1.00 68.26	B
ATOM	3507	N	GLY E		13.970	24.153	56.554	1.00 74.13	В
ATOM	3508	CA	GLY F		12.991	25.206	56.319	1.00 77.67	В
ATOM	3509	C	GLY E		13.580	26.609	56.274	1.00 78.87	
ATOM	3510	ŏ	GLY E		13.815				В
ATOM	3511	N	GLN E		13.813	27.164	55.198	1.00 79.92	В
ATOM	3512		GLN E			27.187	57.444	1.00 78.05	В
		CA			14.379	28.525	57.529	1.00 77.99	В
ATOM	3513	CB	GLN E		14.347	29.002	58.978	1.00 86.19	В
ATOM	3514	CG	GLN E		14.416	30.511	59.179	1.00 95.99	В
ATOM	3515	CD	GLN E		13.097	31.198	58.859	1.00100.91	В
MOTA	3516		GLN E		12.753	32.222	59.459	1.00103.29	. B
MOTA	3517		GLN E		12.353	30.642	57.900	1.00103.10	В
ATOM	3518	C	GLN E	262	15.821	28.546	57.034	1.00 73.93	В
MOTA	3519	0	GLN E	262	16.688	27.869	57.592	1.00 74.56	В
MOTA	3520	И	VAL E	263	16.073	29.318	55.984	1.00 67.20	В
ATOM	3521	CA	VAL E	263	17.421	29.435	55.456	1.00 61.21	, B
ATOM	3522	CB	VAL E		17.400	29.914	53.998	1.00 55.97	'B
ATOM	3523	CG1	VAL E		18.815	30.121	53.502	1.00 52.05	В
ATOM	3524		VAL E		16.661	28.905	53.126	1.00 48.38	В
ATOM	3525	C	VAL E		18.133	30.452	56.336	1.00 60.58	В
ATOM	3526	ō	VAL E		17.505	31.348	56.869		
ATOM	3527	N	THR E		19.440	30.330	56.485		В
ATOM	3528	CA	THR E		20.157			1.00 59.49	В
ATOM	3529	CB	THR E			31.245	57.353	1.00 59.72	В
ATOM	3530	OG1			20.328	30.581	58.696	1.00 57.63	В
ATOM			THR E		19.035	30.191	59.170	1.00 54.09	В
	3531	CG2	THR E		21.008	31.500	59.679	1.00 52.49	В
MOTA	3532	C	THR E		21.513	31.664	56.807	1.00 65.90	В
ATOM	3533	0	THR E		22.200	30.880	56.161	1.00 69.63	В
ATOM	3534	N	ALA E		21.903	32.905	57.074	1.00 70.04	В
ATOM	3535	CA	ALA E	265	23.178	33.427	56.585	1.00 71.83	В
ATOM	3536	CB	ALA E		23.352	34.872	57.019	1.00 73.16	В
MOTA	3537	С	ALA E	265	24.373	32.610	57.050	1.00 72.52	В
MOTA	3538	0	ALA E	265	24.316	31.917	58.071	1.00 72.83	В
ATOM	3539	N	GLY E	266	25.459	32.709	56.289	1.00 73.95	В
ATOM	3540	CA	GLY E	266	26.676	31.987	56.617	1.00 74.15	В
MOTA	3541	C	GLY E		27.294	31.306	55.411	1.00 72.00	В
ATOM	3542	ō	GLY E		26.840	31.486	54.276	1.00 71.05	В.
ATOM	3543	N	ASN E		28.331	30.514	55.651	1.00 70.46	В
ATOM	3544	CA	ASN E		28.991	29.805	54.565		
ATOM	3545	CB	ASN E		30.467			1.00 69.21	В
ATOM	3546	CG	ASN E			29.577	54.895	1.00 75.46	В
ATOM			ASN E	201	31.303	30.827	54.705	1.00 82.33	В
HIOM.	3547	CDT	WOW F	401	32.526	30.807	54.865	1.00 85.69	В

ATOM	3548	ND2	ASN	В	267	30.647	31.925	54.353	1.00	82.59	В
MOTA	3549	C	ASN	В	267	28.336	28.465	54.227		64.44	В
MOTA	3550	0	ASN	В	267	27.702	27.825	55.071	1.00	56.70	В
MOTA	3551	N	VAL	В	268	28.490	28.067	52.970	1.00	61.46	. в
MOTA	3552	CA	VAL	В	268	27.956	26.812	52.473	1.00	60.68	В
ATOM	3553	CB	VAL	в	268	26.757	27.041	51.537		60.04	В
ATOM	3554	CG1	VAL	В	268	26.255	25.714	50.999	1.00	59.59	В
ATOM	3555	CG2	VAL	в	268	25.648	27.747	52.283		61.81	В
ATOM	3556	C	VAL	в	268	29.070	26.129	51.692		60.85	В
ATOM	3557	0	VAL	в :	268	29.458	26.579	50.614		61.07	В
MOTA	3558	N	GLN			29.604	25.056	52.256		60.59	В
ATOM	3559	CA	GLN	в :	269	30.673	24.312	51.610		63.15	В
MOTA	3560	CB	GLN	в	269	31.962	24.442	52.420		65.20	В
ATOM	3561	CG	GLN	В	269	32.707	25.751	52.213	1.00	71.77	В
ATOM	3562	CD	GLN	В	269	33.842	25.943	53.215	1.00	79.78	В
ATOM	3563	OE1	GLN	в :	269	34.648	25.038	53.445		82.19	. B
MOTA	3564	NE2	GLN	в :	269	33.912	27.132	53.811	1.00	82.36	В
ATOM	3565	C	GLN	В :	269	30.280	22.847	51.460	1.00	64.59	В
MOTA	3566	0	GLN	В 2	269	29.470	22.326	52.235	1.00	65.27	. в
ATOM	3567	N	SER			30.835	22.182	50.454	1:00	64.78	В
ATOM	3568	CA	SER			30.504	20.782	50.240	1.00	63.48	В
ATOM	3569	CB	SER			29.104	20.660	49.647	1.00	63.53	В
MOTA	3570	OG	SER :	в :	270	28.762	19.296	49.496	1.00	69.22	В
MOTA	3571	C	SER	в :	270	31.489	20.001	49.379	1.00	61.80	В
ATOM	3572	0	SER	В :	270	32.125	20.540	48.466	1.00	64.03	В
ATOM	3573	И	ILB :			31.601	18.713	49.693	1.00	59.47	В
ATOM	3574	CA	ILE :			32.490	17.788	48.996	1.00	52.99	В
ATOM	3575	CB	ILE :	в :	271	33.538	17.241	49.961	1.00	56.46	В
MOTA	3576	CG2	ILE :			34.727	18.210	50.031	1.00	58.27	В
MOTA	3577	CG1	ILE :			32.887	17.018	51.333	1.00	55.39	В
MOTA	3578	CD1				33.877	16.834	52.480	1.00	58.16	В
ATOM	3579	C	ILE :			31.667	16.650	48.418	1.00	46.51	В
MOTA	3580	0	ILE :			30.938	15.965	49.131	1.00	46.11	В
MOTA	3581	N	ILE :			31.781	16.478	47.108		41.88	В
ATOM	3582	CA	ILE :			31.045	15.456	46.381		37.01	В
ATOM	3583	CB	ILE :			30.093	16.101	45.356		36.10	В
ATOM	3584	CG2	ILE :			29.288	15.039	44.625		32.58	В
ATOM	3585	CG1	ILE :			29.144	17.053	46.077		44.11	В
ATOM	3586	CD1	ILE :			28.227	17.828	45.141		51.23	В
MOTA	3587	C	ILE :			31.976	14.520	45.626		36.59	В
ATOM	3588	0	ILE :			32.981	14.935	45.049		35.79	В
MOTA	3589	N	GLY :			31.636	13.246	45.614		35.00	В
MOTA	3590	CA	GLY :			32.470	12.323	44.892		36.20	В
MOTA	3591	C	GLY :			31.851	12.043	43.552		36.68	В
MOTA	3592	0	GLY			30.631	11.849	43.459		36.92	В
MOTA	3593	N	VAL :				12.059			34.01	В
ATOM	3594	CA	VAL			32.205 32.517	11.746 12.857	41.175		30.90	В
ATOM	3595	CB	VAL			31.669		40.150		29.36	В
	3596		VAL :				12.638	38.903		26.39	В
ATOM ATOM	3597		VAL :			32.215	14.227 10.481	40.732		26.01	В
ATOM	3598	C	VAL :			32.952		40.798		32.12	В
ATOM	3599	O N	THR			34.173	10.485	40.694		32.10	В
ATOM	3600	N	THR			32.208 32.785	9.395 8.102	40.619		34.67	В
MOTA	3601	CA	THR				7.017	40.289		36.64	. В
ATOM	3602	CB	THR			32.257	7.017	41.250		38.71	B
ATOM	3603		THR :			32.759	5.612	42.559		43.63	В
	3604		THR			32.691	7.649	40.806		43.32	В
MOTA	3605	C	TUK.	، د	415	32.511	7.043	38.866	T.00	35.82	В

MOTA	3606	0	THR			31.380	7.318	38.519	1.00	36.62	В
MOTA	3607	N	PHE	В	276	33.562	7.619	38.055	1.00	35.05	В
ATOM	3608	CA	PHE	В	276	33.455	7.174	36.676	1.00	31.86	В
MOTA	3609	CB	PHE	В	276	34.567	7.801	35.826	1.00	30.13	В
ATOM	3610	CG	PHE	В	276	34.369	9.254	35.565	1.00	31.90	В
MOTA	3611	CD1	PHE	В	276	34.760	10.202	36.499	1.00	32.35	В
ATOM	3612	CD2	PHE	В	276	33.716	9.678	34.404	1.00	36.57	В
MOTA	3613	CEl	PHE	В	276	34.501	11.566	36.287	1.00	37.33	В
MOTA	3614	CE2	PHE	В	276	33.449	11.036	34.178	1.00	35.47	В
ATOM	3615	CZ	PHE	В	276	33.842	11.982	35.124	1.00	36.46	В
ATOM	3616	С	PHE	В	276	33.555	5.652	36.625	1.00	30.15	В
ATOM	3617	0	PHE	В	276	34.536	5.069	37.083	1.00	27.92	В
ATOM	3618	N	VAL	В	277	32.534	5.015	36.066	1.00	29.51	В
ATOM	3619	CA	VAL			32.521	3.570	35.975	1.00	29.22	В
MOTA	3620	CB	VAL	В	277	31.138	3.014	36.283	1.00	32.02	В
MOTA	3621	CG1	VAL	В	277	31.212	1.509	36.404	1.00	29.01	В
ATOM	3622		VAL			30.613	3.637	37.566		30.27	В
ATOM	3623	C	VAL	В	277	32.934	3.099	34.603	1.00	28.19	В
ATOM	3624	0	VAL	В	277	32.370	3.522	33.610	1.00	27.93	В
MOTA	3625	N	TYR			33.926	2.214	34.571		30.01	В
ATOM	3626	CA	TYR	В	278	34.462	1.663	33.337		28.31	В
ATOM	3627	СВ	TYR			35.967	1.476	33.452	1.00	25.77	В
ATOM	3628	CG	TYR	В	278	36.704	2.778	33.527	1.00	22.97	В
MOTA	3629		TYR			36.689	3.534	34.694		18.95	В
ATOM	3630	CE1				37.353	4.776	34.762	_	24.89	В
ATOM	3631	CD2	TYR			37.396	3.277	32.414		18.84	В
ATOM	3632	CE2	TYR			38.058	4.504	32.468		25.97	В
ATOM	3633	CZ	TYR			38.036	5.252	33.654		28.43	В
ATOM	3634	OH	TYR			38.721	6.450	33.745		27.64	. В
ATOM	3635	C	TYR			33.855	0.352	32.936		30.69	В
ATOM	3636	ō	TYR			33.704	-0.550	33.761		31.74	В
ATOM	3637	N	GLN			33.516	0.248	31.654		31.66	В
MOTA	3638	CA	GLN	В	279	32.929	-0.981	31.136	1.00	33.20	В
ATOM'	3639	CB	GLN	В	279	32.192	-0.707	29.823	1.00	25.85	В
MOTA	3640	CG	GLN	В	279	31.515	-1.947	29.271	1.00	29.79	В
ATOM	3641	CD	GLN	В	279	30.952	-1.770	27.867	1.00	39.78	В
ATOM	3642	OE1	GLN	В	279	30.094	-2.559	27.445	1.00	42.77	В
ATOM	3643	NE2	GLN	В	279	31.440	-0.756	27.127	1.00	29.64	В
MOTA	3644	C	GLN	В	279	33.999	-2.077	30.932	1.00	33.35	В
MOTA	3645	0	GLN	В	279	33.714	-3.246	31.263	1.00	36.20	В
MOTA	3646	OXT	GLN	В	279	35.109	-1.764	30.445	1.00	28.25	В
MOTA	3647	С	GLY	С	1	82.284	93.643	198.276	1.00	47.80	C
MOTA	3648	0	GLY	С	1	82.098	92.491	197.905	1.00	52.86	C
MOTA	3649	N	GLY	С	1	84.585	94.037	198.871	1.00	52.40	С
MOTA	3650	CA	GLY	С	1	83.542	94.367	197.873	1.00	49.51	С
MOTA	3651	N	VAL	С	2	81.435	94.295	199.063	1.00.	42.64	С
MOTA	3652	CA	VAL.	C	2	80.189	93.678	199.493	1.00	37.51	C
MOTA	3653	CB	VAL	С	2	79.977	93.837	201.003	1.00	34.81	С
ATOM	3654.	CG1	VAL	С	2	78.587	93.368	201.366	1.00	37.50	С
MOTA	3655	CG2	VAL	C	2	81.021	93.025	201.772	1.00	27.99	С
MOTA	3656	C	VAL	С	2	79.038	94.322	198.738	1.00	37.64	C
MOTA	3657	0	VAL		2	78.920		198.713	1.00	37.96	C
MOTA	3658	N	ALA		3	78.197		198.105		39.34	C
ATOM	3659	CA	ALA		3	77.072		197.327		35.95	С
MOTA	3660	CB	ALA		3	77.373		195.857		30.78	C
ATOM	3661	C	ALA		3	75.717		197.609		33.14	C
ATOM	3662	ō	ALA		3	75.601		197.864		37.44	C
MOTA	3663	N	LEU		4	74.689		197.568		30.88	C

MOTA	3664	CA	LEU	С	4	73.339	93.782	197.788	1.00 29.83	С
MOTA	3665	CB	LEU	C	4	72.447	94.942	198.210	1.00 27.49	C
MOTA	3666	CG	LEU	C	4	72.827	95.684	199.485	1.00 21.82	C.
MOTA	3667	CDI	LEU	C	4	71.697	96.632	199.872	1.00 20.80	C
ATOM	3668	CD2	LEU	C	4	73.091	94.693	200.575	1.00 18.02	C
MOTA	3669	C	LEU	C	4	72.830	93.199	196.474	1.00 31.65	C
ATOM	3670	O	LEU	C	4	73.256	93.636	195.391	1.00 32.97	C
ATOM	3671	N	GLY	C	5	71.920	92.228	196.577	1.00 29.09	C
MOTA	3672	CA	GLY	C	5	71.356	91.580	195.402	1.00 23.89	С
ATOM	3673	C	GLY	С	5	70.178	92.295	194.771	1.00 26.39	C
ATOM	3674	0	GLY	C	5	69.595	91.796	193.829	1.00 34.76	. С
ATOM °	3675	N	ALA	C	6	69.807	93.457	195.287	1.00 27.47	C
ATOM	3676	CA	ALA	C	16	68.706	94.232	194.715	1.00 28.27	С
MOTA	3677	CB	ALA	С	6	67.398	93.854	195.371	1.00 24.07	C
ATOM	3678	С	ALA	С	6	68.986	95.709	194.949	1.00 28.88	C
ATOM	3679	0	ALA	С	6	69.741	96.064	195.847	1.00 37.35	C
ATOM	3680	N	THR	C	7	68.381	96.574	194.157	1.00 22.34	C
ATOM	3681	CA	THR	C	7	68.588	97.996	194.333	1.00 21.97	С
ATOM	3682	CB	THR	C	7	68.821	98.709	192.985	1.00 22.33	C
ATOM.	3683	OG1	THR	C	7	67.610	98.704	192.208	1.00 16.75	C
MOTA	3684	CG2	THR	C	7	69.964	98.022	192.215	1.00 15.39	C
ATOM	3685	С	THR	C	7	67.382	98.605	195.014	1.00 26.64	C
ATOM	3686	0	THR	C	7	67.234	99.826	195.062	1.00 28.57	C
MOTA	3687	N	ARG	C	8	66.510		195.523	1.00 29.51	C
ATOM .	3688	CA	ARG	C	8	65.297	98.161	196.232	1.00 29.70	C
ATOM	3689	CB	ARG	C	8	64.341	98.940	195.329	1.00 22.70	C
ATOM	3690	CG	ARG	C	8	63.508	98.056	194.400	1.00 25.09	С
ATOM	3691	CD	ARG	C	8	63.740	98.379	192.936	1.00 24.16	C
MOTA	3692	NE	ARG	C	8	63.441	99.779	192.632	1.00 23.82	C
ATOM	3693	CZ	ARG	C	8	64.368	100.712	192.443	1.00 19.89	C
MOTA	3694	NH1	ARG.	C	8	64.009	101.953	192.177	1.00 20.93	C
MOTA	3695	NH2	ARG	С	8	65.651	100.392	192.505	1.00 12.20	C
MOTA	3696	C	ARG	C	8	64.574	96.922	196.752	1.00 30.90	C
MOTA	3697	0	ARG	C	8	64.866	95.795	196.361	1.00 31.96	C
ATOM	3698	N	VAL	C	9	63.621	97.143	197.637	1,00 31.14	C
MOTA	3699	CA	VAL		9	62.881	96.059	198.222	1.00 27.86	· C
ATOM	3700	CB	VAL	C	9	63.436		199.588	1.00 23.41	C
ATOM	3701	CG1	VAL	С	9	62.515	94.790	200.300	1.00 31.32	C
ATOM	3702	CG2	VAL		9	64.789	95.086	199.433	1.00 25.66	C
ATOM	3703	C	VAL		9	61.430	96.469	198.364	1.00 31.99	C
MOTA	3704	0	VAL		9	61.113	97.600	198.750	1.00 29.12	C
MOTA	3705	N	ILE		10	60.551	95.541	198.006	1.00 34.65	C
MOTA	3706	CA	ILE		10	59.131	95.764	198.121	1.00 32.90	C
ATOM	3707	CB	ILE		10	58.405		196.862	1.00 25.94	C
MOTA	3708	CG2	ILE		10	56.918		197.035	1.00 23.95	C
ATOM	3709		ILE		10	58.895			1.00 26.72	С
ATOM	3710		ILE		10	58.573		195.857	1.00 23.90	C
MOTA	3711	C	ILE		10	58.665		199.262	1.00 36.81	C
ATOM	3712	0	ILE		10	58.809		199.220	1.00 34.85	С
ATOM	3713	N	TYR		11	58.143		200.300	1.00 38.74	C
ATOM	3714	CA	TYR		11	57.644		201.451	1.00 39.72	C
ATOM	3715	CB	TYR		11	58.020		202.755	1.00 35.97	C
MOTA	3716	CG	TYR		11	58.011		203.926	1.00 40.02	C
MOTA	3717		TYR		11	59.179		204.327	1.00 42.31	С
ATOM	3718		TYR		11	59.184		205.382	1.00 41.14	С
ATOM	3719	CD2			11	56.833		204.612	1.00 35.73	C
MOTA	3720		TYR		11	56.827		205.669	1.00 37.89	C
MOTA	3721	CZ	TYR	C	11	58.012	92.713	206.045	1.00 39.50	Ċ

ATOM	3722	OH	TYR C	11	58.037	91.789 207.065	1.00 38.93	C
MOTA	3723	C	TYR C	11	56.130	94.737 201.353	1.00 39.73	C
ATOM	3724	0	TYR C	11	55.454	95.749 201.560	1.00 32.07	C
ATOM	3725	N	PRO C	12	55.581	93.546 201.024	1.00 42.99	C
MOTA	3726	CD	PRO C	. 12	56.323	92.335 200.634	1.00 42.10	Č
ATOM	3727	CA	PRO C		54.135	93.319 200.890	1.00 42.62	Č
ATOM	3728	CB	PRO C		54.051	91.920 200.271	1.00 41.25	Č
ATOM	3729	CG	PRO C		55.403	91.728 199.619	1.00 41.11	Č
ATOM	3730	C	PRO C		53.489	93.355 202.258	1.00 39.78	Č
ATOM	3731	ō	PRO C		53.844	92.558 203.123	1.00 37.52	C
ATOM	3732	N	ALA C		52.559	94.279 202.465	1.00 42.06	C
ATOM	3733	CA	ALA C		51.891	94.360 203.756	1.00 47.94	c
ATOM	3734	CB	ALA C		50.793	95.409 203.719	1.00 47.72	
MOTA	3735	CD	ALA C		51.310	92.983 204.095	1.00 47.72	C
ATOM	3736	Ö	ALA C		50.589	92.377 203.292	1.00 52.52	
ATOM	3737	N	GLY C		51.645			C
ATOM	3738	CA	GLY C		51.150	92.484 205.279 91.188 205.691	1.00 55.11	C
ATOM	3739	C	GLY C		52.262		1.00 55.68	C
ATOM	3740	Ö	GLY C		52.311	90.167 205.801 89.412 206.774	1.00 58.97	C
ATOM			GLN C				1.00 60.10	C
	3741	N	GLN C		53.152	90.137 204.809	1.00 59.01	C
ATOM	3742	CA			54.267	89.194 204.806	1.00 58.86	C
MOTA	3743	CB	GLN C		55.280	89.563 203.722	1.00 60.40	C
ATOM '	3744	CG	GLN C		54.695	89.693 202.329	1.00 68.08	C
ATOM	3745	CD	GLN C		54.804	88.425 201.503	1.00 72.86	C
ATOM	3746	OE1	GLN C		54.378	87.353 201.929	1.00 76.38	C
ATOM	3747	NE2	GLN C		55.372	88.546 200.304	1.00 75.46	C
ATOM	3748	C	GLN C		54.952	89.223 206.163	1.00 60.53	C
ATOM	3749	0	GLN C		55.174	90.285 206.741	1.00 61.41	C
MOTA	3750	N	LYS C		55.280	88.053 206.682	1.00 63.48	C
MOTA	3751	CA	LYS C		55.945	87.996 207.968	1.00 66.28	C
ATOM	3752	CB	LYS C	16	55.995		1.00 72.55	C
MOTA	3753	CG	LYS C	16	56.490	86.423 209.906	1.00 81.73	С
MOTA	3754	CD	LYS C		56.700	84.956 210.296	1.00 89.61	С
ATOM	3755	CE	LYS C		55.530	84.061 209.847	1.00 92.46	C
ATOM	3756	NZ	LYS C		54.196	84.530 210.332	1.00 92.32	C
ATOM	3757	C	LYS C		57.364	88.524 207.808	1.00 66.00	C
MOTA	3758	0	LYS C		57.938	89.067 208.747	1.00 69.14	С
ATOM	3759	N	GLN C		57.922	88.374 206.609	1.00 62.74	C
ATOM	3760	CA	GLM C		59.287	88.819 206.349	1.00 59.20	C
MOTA	3761	CB	GLN C		60.260	87.982 207.173	1.00 58.18	C
MOTA	3762	CG	GLN C		60.110	86.513 206.890	1.00 62.51	· C
ATOM	3763	CD	GLN C		61.372	85.733 207.151	1.00 65.45	C
MOTA	3764		GLM C		61.894	85.727 208.274	1.00 62.42	C
MOTA	3765	NE2	GLN C		61.878	85.060 206.109	1.00 62.28	C
MOTA	3766	С	GLN C		59.704	88.728 204.878	1.00 53.91	C
ATOM	3767	0	GLN C		59.260	87.852 204.145	1.00 53.08	C
MOTA	3768	N	VAL C		60.569	89.643 204.460	1.00.48.87	С
ATOM	3769	CA	VAL C		61.064	89.648 203.099	1.00 45.24	C
MOTA	3770	CB	VAL C	18	60.771	90.964 202.399	1.00 44.20	. С
MOTA	3771		VAL C		61.381	90.956 201.016	1.00 45.77	C
MOTA	3772	CG2	VAL C	18	59.276	91.170 202.307	1.00 48.76	C
MOTA	3773	C	VAL C	18	62.562	89.468 203.211	1.00 47.01	C
ATOM	3774	0	VAL C	18	63.167	89.863 204.206	1.00 49.52	C
MOTA	3775	N	GLN C	19	63.175	88.871 202.203	1.00 44.25	C
MOTA	3776	CA	GLN C	19	64.597	88.658 202.287	1.00 43.81	C
ATOM	3777	CB	GLN C		64.881	87.169 202.383	1.00 47.35	Ċ
MOTA	3778	CG	GLN C		64.106	86.340 201.401	1.00 58.37	č
MOTA	3779	CD	GLN C		64.022	84.901 201.837	1.00 60.14	č

MOTA	3780	OE1	GLN C	19	63.414	84.597 202.863	1.00 63.64	C
MOTA	3781	NE2	GLN C	19	64.640	84.005 201.069	1.00 66.29	C
MOTA	3782	C	GLN C	19	65.369	89.292 201.156	1.00 40.82	C
ATOM	3783	0	GLN C	19	64.862	89.439 200.059	1.00 39.81	C
MOTA	3784	N .	LEU C	20	66.601	89.685 201.471	1.00 37.67	· C
MOTA	3785	CA	LEU C	20	67.517	90.334 200.548	1.00 32.34	C
MOTA	3786	CB	LEU C	20	67.717	91.790 200.983	1.00 27.58	C
MOTA	3787	CG	LEU C	20	68.627	92.722 200.172	1.00 27.41	C
MOTA	3788	CD1	LEU C	20	68.004	93.002 198.819	1.00 23.64	C
MOTA	3789	CD2	LEU C	20	68.838	94.024 200.934	1.00 26.17	C
MOTA	3790	C	LEU C		68.855	89.577 200.572	1.00 32.15	C
MOTA	3791	0	LEU C		69.261	89.047 201.601	1.00 28.32	C
MOTA	3792	N	ALA C		69.535	89.531 199.434	1.00 34.28	Ċ
ATOM	3793	CA	ALA C		70.799	88.820 199.346	1.00 32.51	Ċ
ATOM	3794	CB	ALA C		70.892	88.071 198.017	1.00 26.24	Č
MOTA	3795	C	ALA C		71.969	89.757 199.469	1.00 33.56	Ċ
MOTA	3796	ō	ALA C		71.919	90.901 199.022	1.00 30.14	Ċ.
MOTA	3797	N	VAL C		73.031	89.243 200.072	1.00 35.99	Ċ.
ATOM	3798	CA	VAL C		74.253	89 998 200.239	1.00 39.04	Ċ
ATOM	3799	CB	VAL C		74.565	90.356 201.691	1.00 37.76	Č
ATOM	3800		VAL C		75.364	91.650 201.728	1.00 33.72	č
ATOM	3801		VAL C		73.304	90.429 202.494	1.00 38.39	č
ATOM	3802	C	VAL C		75.334	89.048 199.829	1.00 43.75	č
ATOM	3803	ō	VAL C		75.321	87.869 200.201	1.00 47.48	Č
ATOM	3804	N	THR C		76.288	89.569 199.086	1.00 44.44	č
ATOM	3805	CA	THR C		77.380	88.760 198.635	1.00 45.58	Č
ATOM	3806	CB	THR C		77.140	88.340 197.189	1.00 47.38	Ċ
ATOM	3807	OG1	THR C		78.369	87.889 196.616	1.00 58.41	Ċ
ATOM	3808	CG2	THR C		76.591	89.501 196.388	1.00 50.41	c
ATOM	3809	c	THR C		78.661	89.568 198.782	1.00 44.89	c
ATOM	3810	õ	THR C		78.683	90.765 198.507	1.00 41.14	c
ATOM	3811	N	ASN C		79.709	88.892 199.249		c
ATOM	3812	CA	ASN C		81.024	89.473 199.470	1.00 44.67	c
ATOM	3813	CB	ASN C		81.499	89.123 200.882	1.00 41.68	C
ATOM	3814	CG	ASN C		82.942	89.541 201.142	1.00 46.70	C
ATOM	3815		ASN C		83.464	90.445 200.490	1.00 48.70	C
ATOM	3816		ASN C		83.585	88.894 202.113	1.00 42.01	C
ATOM	3817	C	ASN C			88.926 198.435	1.00 47.88	
ATOM	3818	0	ASN C		82.000	87.741 198.451	1.00 47.88	C
ATOM	3819	И	ASN C		82.336 82.446	89.807 197.542	1.00 52.95	C
ATOM	3820	CA	ASN C		83.385	89.477 196.460	1.00 56.72	C C
ATOM	3821	CB	ASN C			90.632 195.461	1.00 53.45	
ATOM	3822	CG	ASN C		83.471		1.00 53.45	. C
ATOM	3823		ASN C		82.174 81.096	90.883 194.750 90.660 195.300	1.00 54.34	
ATOM	3824		ASN C		82.265	91.372 193.521	1.00 56.79	C
	3825	C ZUNZ			84.802		1.00 58.79	C C
ATOM		-	ASN C			89.194 196.933 88.155 196.624	1.00 58.94	-
ATOM	3826	0	ASN C		85.382			C
ATOM	3827 3828	N	ASP C		85.360	90.149 197.661 90.046 198.159	1.00 59.08 1.00 61.73	C
ATOM		CA			86.714			C
ATOM	3829	CB	ASP C		86.929	91.072 199.250	1.00 65.93	C
ATOM	3830	CG	ASP C		86.784	92.482 198.741	1.00 67.09	C
MOTA	3831		ASP C		86.874	93.410 199.573	1.00 70.36	C
ATOM	3832		ASP C		86.581	92.658 197.513	1.00 65.25	C
ATOM	3833	C	ASP C		87.110	88.679 198.654	1.00 63.97	C
MOTA	3834	0	ASP C		86.846	88.308 199.793	1.00 65.66	C
ATOM	3835	N	GLU C		87.771	87.942 197.775	1.00 67.29	C
ATOM	3836	CA	GLU C		88.231	86.599 198.067	1.00 70.86	C
MOTA	3837	CB	GLU C	27	89.165	86.126 196.945	.1.00 77.52	C -

MOTA	3838	CG	GLU	C	27	88.407	85.691	195.682	1.00 91.83	C
ATOM	3839	CD	GLU	С	27	89.160	85.953	194.379	1.00 98.28	С
ATOM	3840	OE1	GLU	С	27	90.337	85.536	194.265	1.00102.35	C
ATOM	3841	OE2			27	88.558		193.465	1.00100.04	č
ATOM	3842	C	GLU		27	88.915		199.414	1.00 69.08	Č
ATOM	3843	ō	GLU		27	88.969		199.977	1.00 69.88	C
MOTA	3844	N								
			ASN		28	89.423		199.951	1.00 69.03	C
ATOM	3845	CA	ASN		28	90.096		201.236	1.00 73.05	C
ATOM	3846	CB	ASN		28	91.540		201.032	1.00 79.79	C
MOTA	3847	CG	ASN		28	92.294		199.977	1.00 84.46	C
MOTA	3848		ASN	С	28	93.371		199.526	1.00 80.13	C
MOTA	3849	ND2	ASN	C	28	91.729		199.583	1.00 86.62	C.
ATOM	3850	C	ASN	C	28	90.076		202.043	1.00 71.95	С
MOTA	3851	0	ASN	C	28	90.868	89.680	201.822	1.00 75.63	C
MOTA	3852	N	SER	С	29	89.159	88.812	202.997	1.00 70.78	,C
MOTA	3853	CA	SER	C	29	88.962	89.951	203.885	1.00 69.08	C
MOTA	3854	CB	SER	С	29	88.990	91.270	203.100	1.00 69.88	С
MOTA	3855	OG	SER	С	29	87.969	91.304	202.118	1.00 62.99	Č
ATOM	3856	C	SER		29	87.588		204.516	1.00 65.21	č
ATOM	3857	o	SER		29	86.578		203.821	1.00 66.37	č
ATOM	3858	N	THR		30	87.549		205.828	1.00 61.05	C
ATOM	3859	CA	THR		30	86.281		206.496	1.00 58.61	c
ATOM	3860	СВ	THR		30	86.486		207.866	1.00 57.95	
ATOM	3861	OG1	THR		30	87.288		207.713		C
									1.00 61.24	C
ATOM	3862	CG2	THR		30	85.163		208.449	1.00 63.15	C
ATOM	3863	C	THR		30	85.561		206.672	1.00 55.48	C
ATOM	3864	0	THR		30	86.173		206.592	1.00 57.77	, C
ATOM	3865	N	TYR		31	84.253		206.885	1.00 51.80	С
MOTA	3866	CA	TYR		31	83.438		207.090	1.00 50.13	C
MOTA.	3867	CB	TYR	С	31	82.756		205.796	1.00 50.26	C
MOTA	3868	CG	TYR	C	31	83.644	92.926	204.802	1.00 52.64	C
MOTA	3869	CD1	TYR	С	31	83.973	92.318	203.595	1.00 52.05	C
MOTA	3870	CE1	TYR	С	31	84.730	92.985	202.646	1.00 56.63	C
MOTA	3871	CD2	TYR	C	31	84.104	94.219	205.037	1.00 55.05	C
ATOM	3872	CE2	TYR	C	31	84.859	94.895	204.094	1.00 56.52	С
MOTA	3873	CZ	TYR	С	31	85.165	94.275	202.903	1.00 59.00	С
MOTA	3874	OH	TYR		31	85.881		201.957	1.00 67.61	Ċ
MOTA	3875	С	TYR	С	31	82.346		208.124	1.00 49.09	Č
MOTA	3876	0	TYR		31	81.870		208.318	1.00 51.62	, Č
ATOM	3877	N	LEU		32	81.957		208.798	1.00 44.10	Ċ
ATOM	3878	CA	LEU		32	80.883		209.762	1.00 41.27	č
ATOM	3879	CB	LEU		32 .	81.241		211.052	1.00 47.86	č
ATOM	3880	CG	LEU		32	81.985		212.111	1.00 50.85	C
ATOM	3881	CD1	LEU		32	82.422		213.240	1.00 52.23	c
ATOM	3882	CD2	LEU		32				1.00 32.23	
		CDZ				81.085		212.621	•	C
MOTA	3883		LEU		32	79.733		209.078	1.00 41.23	
ATOM	3884	0	LEU		32	79.837		208.689	1.00 36.29	C
MOTA	3885	N	ILE		33	78.644		208.896	1.00 38.59	C
MOTA	3886	CA	ILE		33	77.491		208.255	1.00 35.09	C
MOTA	3887	CB	ILE		33	76.791		207.392	1.00 37.49	. С
MOTA	3888	CG2			33	75.614		206.630	1.00 35.15	C
MOTA	3889		ILE		33	77.819	91.425	206.447	1.00 38.22	C
MOTA	3890	CD1	ILE	C	33	78.638		205.654	1.00 27.16	C
MOTA	3891	C	ILE	C	33	76.565	93.600	209.340	1.00 35.31	C
MOTA	3892	0	ILE	C	33	76.190		210.243	1.00 34.27	С
ATOM	3893	N	GLN		34	76.216		209.249	1.00 33.45	C
ATOM	3894	CA	GLN		34	75.324		210.207	1.00 34.45	C
ATOM	3895	CB	GLN		34	76.099		211.019	1.00 38.51	Ċ
								-		

MOTA	3896	CG	GLN	С	34	75.587	96.769	212.409	1.00	38.42	C
MOTA	3897	CD	GLN	C	34	76.488	97.705	213.177	1.00	42.59	C
MOTA	3898	OE1	GLN	С	34	76.633	98.874	212.825	1.00	49.60	С
MOTA	3899	NE2	GLN	С	34	77.115	97.193	214.226	1.00	44.72	C
MOTA	3900	С	GLN	С	34	74.249	96.181	209.373	1.00	32.15	С
MOTA	3901	0	GLN	С	34	74.546	97.088	208.605	1.00	31.59	C
ATOM	3902	N	SER	С	35	73.003	95.748	209.526	1.00	30.76	C
ATOM	3903	CA	SER		35	71.911		208.746		32.03	· c
ATOM	3904	CB	SER		35	71.287		207.892		33.64	č
ATOM	3905	OG	SER	-	35	72.294		207.296		41.25	č
MOTA	3906	C	SER		35	70.815		209.573		29.68	č
ATOM	3907	ō	SER		35	70.572		210.706		36.57	č
MOTA	3908	N	TRP	-	36	70.145		208.999		24.09	c
ATOM	3909	CA	TRP		36	69.044		209.689		27.31	C
	3910	CB	TRP		36	69.550		210.738		18.33	C
MOTA		CG	TRP		36		100.862			19.19	c
MOTA	3911										
ATOM	3912	CD2	TRP		36			209.738		20.58	C
MOTA	3913	CE2	TRP		36		102.380			24.78	
MOTA	3914	CE3	TRP		36			209.699		17.43	C
ATOM	3915		TRP		36		102.042			24.90	C
ATOM	3916	NE1			36		102.965			26.58	C
ATOM	3917	CZ2	TRP		36		102.905			18.18	C
ATOM	3918	CZ3			36		100.749			19.76	C
ATOM	3919	CH2	TRP		36		102.076			18.14	C
ATOM	3920	C	TRP		36	68.160		208.683		27.98	C
ATOM	3921	0	TRP		36	68.480		207.502		27.18	· C
ATOM	3922	N	VAL		37	67.035	•	209.163		26.68	C
ATOM	3923	CA	VAL		37		100.536			27.00	C
ATOM	3924	CB	VAL		37	64.882		208.016		24.02	C
ATOM	3925		VAL		37		100.408			27.07	C
ATOM .	3926		VAL		37	65.310		207.385		25.57	C
MOTA	3927	C,	VAL		37		101.830			27.29	C
ATOM	3928	0	VAL		37		101.838			33.48	C
ATOM	3929	N	GLU		38		102.925			25.74	C
ATOM	3930	CA	GLU		38		104.230			27.08	C
ATOM	3931	CB	GLU		38		105.265			24.24	C
ATOM	3932	CG	GLU		38		104.944			30.81	C
MOTA	3933	CD	GLU		38		105.798			32.52	C
ATOM	3934		GLU		38		106.849			27.54	C
MOTA	3935		GLU		38		105.428			30.88	C
ATOM	3936	C	GLU		38		104.538			27.46	C
ATOM	3937	0	GLU		38		103.940			29.90	C
ATOM	3938	N	ASN		39		105.433	208.563		27.37	C
MOTA	3939	CA	ASN		39		105.789			28.73	C
ATOM	3940	CB	ASN		39		106.202			30.19	C
MOTA	3941	CG	ASN		39			209.695		41.20	C
ATOM	3942		ASN		39			209.247		41.54	C
ATOM	3943		ASN		39			210.841		41.71	C
ATOM	3944	C	ASN		39			206.961		32.17	C
ATOM	3945	0	ASN		39			206.799		28.30	C
MOTA	3946	N	ALA		40			206.332		34.05	C
ATOM	3947	CA	ALA		40			205.353		34.87	C
ATOM	3948	CB	ALA		40			204.906		39.82	C
MOTA	3949	C	ALA		40			205.861		37.43	C
ATOM	3950	0	ALA		40			205.123		41.98	C
ATOM	3951	N	ASP		41			207.122		39.93	C
ATOM	3952	CA	ASP		41			207.655		43.39	C
MOTA	3953	CB	ASP	C	41	62.053	111.746	208.851	T.00	47.27	C

MOTA	3954	CG	ASP	С	41	60.762	112.410	208.455	1.00	52.51	С
ATOM	3955	OD1	ASP	C	41	60.797	113.241	207.521	1.00	57.76	C
ATOM	3956	OD2	ASP	C	41		112.105		1.00	50.84	C
ATOM	3957	C	ASP		41	64.236	110.878	208 027	1.00		Ċ
ATOM	3958	ō	ASP		41		111.756			48.94	Č
ATOM	3959	N	GLY		42		109.649				
										40.84	C
MOTA	3960	CA	GLY		42		109.322			34.57	С
ATOM	3961	С	GLY		42		108.859		1.00	36.10	С
MOTA	3962	0	GLY	C	42		108.572		1.00	34.98	С
MOTA	3963	N	VAL	C	43	65.188	108.771	210.344	1.00	37.80	С
MOTA	3964	CA	VAL	C	43	65.374	108.330	211.719	1.00	38.56	C
ATOM	3965	CB	VAL	C	43	64.458	109.106	212.709	1.00	31.38	С
ATOM	3966		VAL		43		110.228			29.16	Č
ATOM	3967		VAL		43		108.176			38.44	Č
ATOM	3968	C	VAL		43		106.824				c
		ō								42.60	
ATOM	3969		VAL		43		106.207			45.76	C
ATOM.	3970	N	LYS		44		106.242			39.87	C
MOTA	3971	CA	LYS		44		104.822			40.62	С
ATOM	3972	CB	LYS		44	67.302	104.330	213.619	1.00	41.67	C
MOTA	3973	CG	LYS	C	44	68.552	104.505	212.777	1.00	43.65	C
MOTA	3974	CD	LYS	C	44	69.558	105.391	213.481	1.00	49.04	C
MOTA	3975	CE	LYS	С	44	70.829	105.539	212.673	1.00	50.04	С
ATOM	3976	NZ	LYS	C	44	71.483	104.222	212,479	1.00	56.49	C
ATOM	3977	C	LYS	C	44		104.472		1.00		· c
ATOM	3978	ō	LYS	_	44		104.319			42.96	č
MOTA	3979	N	ASP		45		104.315		1.00		C
			ASP								
MOTA	3980	CA			45		103.957		1.00		C
ATOM	3981	CB	ASP		45		104.457		1.00		Ċ
ATOM	3982	CG	ASP		45	•	104.342		1.00		C
MOTA ·	3983		ASP		45	61.558	103.415	211.825	1.00	42.26	C.
ATOM	3984	OD2	ASP	С	45 ·	60.234	105.175	211.899	1.00	35.65	С
ATOM	3985	C	ASP	C	45	62.647	102.457	214.210	1.00	45.07	C
ATOM	3986	0	ASP	С	45	63.520	101.955	213.490	1.00	50.93	C
ATOM	3987	N	GLY	С	46	61.757	101.719	214.843	1.00	44.81	C
ATOM	3988	CA	GLY		46		100.279		1.00		Ċ
ATOM	3989	C	GLY		46	60.863		213.809	1.00		Č
ATOM	3990	ō	GLY		46	60.587	•	213.911	1.00		Č
MOTA	3991	N	ARG		47		100.477				
									1.00		C
MOTA	3992	CA	ARG		47	59.293		212.002	1.00		C
ATOM	3993	CB	ARG		47		101.035		1.00		C
MOTA	3994	CG	ARG		47		101.670		1.00		С
ATOM	3995	CD	ARG		47		102.519		1.00	68.87	C
ATOM	3996	NE	ARG	С	47		102.988	212.711	1.00	82.07	C
MOTA	3997	cz	ARG	С	47	55.298	102.235	213.265	1.00	90.71	C
ATOM	3998	NH1	ARG	C	47	55.562	100.980	213.604	1.00	95.97	. C
ATOM	3999	NH2	ARG	C	47	54.082	102.729	213.476	1.00	94.06	С
ATOM	4000	С	ARG		47	59.700	98.685	211.329	1.00		C
ATOM	4001	ō	ARG		47	58.876		211.122	1.00		Č
ATOM	4002	N	PHE		48	60.976		210.993	1.00		Č
ATOM	4003	CA	PHE		48			210.353		39.64	
	4003	CB	PHE			61.445			1.00		C
ATOM					48	61.660		208.839			C
MOTA	4005	CG	PHE		48	60.389		208.084	1.00		C
MOTA	4006		PHE		48	59.823		207.973	1.00		Ç
MOTA	4007		PHE		48	59.691	96.656	207.590	1.00		· C
MOTA	4008	CE1	PHE	C	48	58.583		207.398	1.00	26.97	C
ATOM	4009	CE2	PHE	С	48	58.447	96.812	207.011	1.00	26.86	С
MOTA	4010	CZ	PHE	С	48	57.886		206.915	1.00		C
ATOM	4011	C	PHE		48	62.723		211.003	1.00		Č
		-		-		•				- -	_

MOTA	4012	0	PHE C	48	63.535	97.681 211.397	1.00 34.61	С
ATOM	4013	N	ILE (49	62.892	95.554 211.106	1.00 35.46	C
ATOM	4014	CA	ILE (49	64.080	94.996 211.716	1.00 37.43	С
ATOM	4015	CB ·	ILE (49	63.723	94.375 213.072	1.00 41.64	C
MOTA	4016	CG2	ILE C	49	64.938	93.703 213.700	1.00 36.12	C
ATOM	4017	CG1	ILE C	49	63.239	95.492 213.999	1.00 42.64	C
MOTA	4018	CD1	ILE C		62.438	94.997 215.178	1.00 50.85	C
ATOM	4019	C	ILE C	49	64.713	93.979 210.789	1.00 36.63	C
ATOM	4020	0	ILE C		64.030	93.183 210.163	1.00 40.23	Č
ATOM	4021	N	VAL C		66.032	94.015 210.705	1.00 32.70	Č
ATOM	4022	CA	VAL C		66.751	93.123 209.820	1.00 33.80	Č
ATOM	4023	CB	VAL C		67.737	93.927 208.927	1.00 37.22	Ċ
ATOM	4024	CG1			68.394	93.013 207.898	1.00 36.52	č
ATOM	4025	CG2	VAL C		67.001	95.074 208.253	1.00 37.37	Ċ
ATOM	4026	C	VAL C		67.543	92.125 210.623	1.00 32.90	Č
MOTA	4027	0	VAL C		68.100	92.472 211.660	1.00 35.67	Ċ
MOTA	4028	N	THR C	51	67.601	90.886 210.153	1.00 29.99	Ċ
MOTA	4029	CA	THR C	51	68.378	89.864 210.845	1.00 30.68	Č
ATOM	4030	CB	THR C	51	67.495	88.848 211.603	1.00 35.47	. Ĉ
ATOM	4031	OG1	THR C	•	66.548	88.268 210.696	1.00 40.09	Ċ
ATOM	4032	CG2	THR C		66.753	89.512 212.744	1.00 40.38	Ċ
ATOM	4033	C	THR C		69.180	89.079 209.831	1.00 32.09	Ċ
MOTA	4034	0	THR C	51	68.758	88.886 208.693	1.00 34.34	Ċ
MOTA	4035	N	PRO C		70.375	88.650 210.220	1.00 31.87	Ċ
ATOM	4036	CD	PRO C		71.052	87.490 209.626	1.00 31.15	Č
ATOM	4037	CA	PRO C		70.900	88.934 211.557	1.00 32.99	Ċ
ATOM	4038	CB	PRO C		72.058	87.947 211.704	1.00 30.92	Č
ATOM	4039	CG	PRO C		72.382	87.552 210.299	1.00 35.51	Ċ
MOTA	4040	C	PRO C		71.362	90.377 211.642	1.00 35.74	Ċ
ATOM	4041	0	PRO C		71.961	90.904 210.710	1.00 39.69	č
ATOM	4042	N	PRO C		71.085	91.043 212.764	1.00 33.93	Ċ
ATOM	4043	CD	PRO C	53	70.457	90.552 214.002	1.00 32.30	C
MOTA	4044	CA	PRO C	53	71.505	92.435 212.898	1.00 32.39	C
ATOM	4045	CB	PRO C		70.969	92.820 214.273	1.00 32.88	Ċ
ATOM	4046	CG	PRO C	53	70.994	91.499 215.023	1.00 29.64	Ċ
ATOM	4047	C	PRO C	53	73.012	92.638 212.784	1.00 32.10	Ċ
MOTA	4048	0	PRO C	53	73.462	93.742 212.516	1.00 31.38	Ċ
ATOM	4049	N	LEU C	54	73.787	91.576 212.985	1.00 34.31	C
MOTA	4050	CA	LEU C		75.247	91.667 212.920	1.00 35.90	C
MOTA	4051	CB	LEU C	54	75.799	92.224 214.226	1.00 36.76	C
MOTA	4052	CG	LEU C	54	77.317	92.330 214.328	1.00 38.09	С
MOTA	4053	CD1	LEU C	54	77.794	93.603 213.622	1.00 43.96	С
MOTA	4054	CD2	LEU C	54	77.714	92.359 215.778	1.00 37.68	C
ATOM	4055	C	LEU C	54	75.872	90.307 212.705	1.00 38.16	С
MOTA	4056	0	LEU C	54	75.654	89.404 213.513	1.00 43.88	C
MOTA	4057	N	PHE C	55	76.663	90.157 211.646	1.00 36.15	С
MOTA	4058	CA	PHE C	55	77.302	88.872 211.359	1.00 35.98	C
ATOM	4059	CB	PHE C	55	76.318	87.917 210.702	1.00 32.13	С
MOTA	4060	CG	PHE C	55	75.825	88.388 209.374	1.00 39.81	С
MOTA	4061	CD1	PHE C	55	76.430	87.959 208.198	1.00 41.92	C
MOTA	4062		PHE C		74.770	89.294 209.294	1.00 42.59	C
MOTA	4063	CEl	PHE C	55	75.993	88.425 206.951	1.00 42.45	Ċ
ATOM	4064	CE2	PHE C		74.325	89.767 208.056	1.00 47.62	Č
MOTA	4065	CZ	PHE C		74.938	89.332 206.880	1.00 44.74	Ċ
ATOM	4066	C	PHE C		78.496	89.032 210.451	1.00 39.55	Č
ATOM	4067	0	PHE C	55	78.666	90.067 209.805	1.00 42.02	Č
MOTA	4068	N	ALA C		79.316	87.990 210.385	1.00 42.81	Č
MOTA	4069	CA	ALA C	56	80.517	88.030 209.558	1.00 41.76	C

MOTA	4070	CB	ALA	C 5	6	81.694		210.356	1.00	38.75	C
MOTA	4071	C	ALA	C 5	6	80.428	87.287	208.223	1.00	40.09	C
MOTA	4072	0	ALA	C 5	6	79.750	86.264	208.084	1.00	37.71	C
MOTA	4073	N	MET	C 5	57	81.111	87.836	207.232	1.00	39.98	C
MOTA	4074	CA	MET	C 5	57	81.167	87.232	205.916	1.00	42.59	C
MOTA	4075	CB	MET	C 5	7	80.494	88.121	204.875	1.00	39.70	C
MOTA	4076	CG	MET	C 5	57	79.028	88.363	205.128	1.00	43.59	С
ATOM	4077	SD	MET	C 5	57	78.096	88.358	203.578	1.00	47.27	. С
MOTA	4078	CE	MET	C 5	57	78.721	89.808	202.864	1.00	57.39	C
MOTA	4079	C	MET	C 5	7	82.656	87.114	205.632	1.00	44.97	C
ATOM	4080	0	MET	C 5	7	83.342	88.116	205.401	1.00	42.67	C
ATOM	4081	N	LYS (C 5	8	83.154		205.679		47.91	C
ATOM	4082	CA	LYS	C 5	8	84.564	85.642	205.450	1.00		C
ATOM	4083	CB	LYS (C 5	8	85.055	84.555	206.403	1.00	61.66	C
ATOM	4084	CG	LYS	C 5	8	86.563	84.497	206.557	1.00	66.16	Ċ
ATOM	4085	CD	LYS		8	86.969		207.466	1.00	71.39	Ċ
ATOM	4086	CE	LYS		8	88.326		208.115	1.00	76.59	Ċ
ATOM	4087	NZ	LYS	C 5	8	88.273		209.061	1.00	75.59	. C
ATOM	4088	C	LYS		8	84.839		204.006	1.00	57.70	C
ATOM	4089	0	LYS (8	84.336		203.535		60.74	Č
ATOM	4090	N	GLY (٠ و	85.641		203.310		57.50	Č
ATOM	4091	CA	GLY (-	9	85.970		201.931		57.28	Ċ
ATOM	4092	C	GLY (9	84.733		201.066		55.51	Č
ATOM	4093	ō	GLY (9	83.659		201.519	1.00	52.74	Ċ
ATOM	4094	N	LYS		0	84.879		199.829		56.19	č
ATOM	4095	CA	LYS		0	83.748		198.914		58.74	č
ATOM	4096	СВ	LYS		· 0	84.178		197.556	1.00	58.13	č
ATOM	4097	CG	LYS		0	85.264		196.874		61.25	č
ATOM	4098	CD	LYS		0	85.233		195.361		64.10	č
ATOM	4099	CE	LYS		0	83.992		194.783	1.00	73.21	Ċ
ATOM	4100	NZ	LYS		0	83.977		193.287		80.41	C
ATOM	4101	C.	LYS		0	82.681		199.529		58.59	Ċ
ATOM	4102	0	LYS		0	82.849		199.624		61.67	Ğ
ATOM	4103	N	LYS		1	81.591		199.959		55.11	Ĉ
ATOM	4104	CA	LYS (1	80.489		200.595		50.13	Ċ
ATOM	4105	CB	LYS		1	80.600		202.117		50.07	Ċ
ATOM	4106	CG	LYS		1	80.714		202.838	1.00	57.49	Ċ
ATOM	4107	CD	LYS		1	79.718		202.030		60.10	G
ATOM	4108	CE	LYS		1	79.980		205.062		68.66	C
ATOM	4109	NZ	LYS		1	78.938		205.062		66.44	c
ATOM	4110	C	LYS		1	79.189		200.136		47.80	c
ATOM	4111	0	LYS		1	79.190		199.462		46.03	C
ATOM	4112	N	GLU (2	78.076		200.497		47.17	c
ATOM		. CA	GLU (2	76.771		200.437		47.93	C
			GLU (2	76.308					c
ATOM ATOM	4114	CB CG	GLU		2	75.526		198.824 197.939		48.27 65.47	Č
	4115				2	74.027					•
MOTA		CD	GLU (2			197.986		72.46	C
MOTA	4117				52 52	73.458		199.101		77.88 72.13	C
ATOM	4118		GLU			73.420		196.899			C
MOTA	4119	C	GLU		2			201.279		45.06	C
MOTA	4120	0	GLU (2	75.842		201.776		50.21	C
ATOM	4121	N	ASN		3	75.054		201.742		39.37	C
ATOM	4122	CA	ASN		3	74 . 136		202.838		38.76	C
ATOM	4123	CB	ASN		3	74.684		204.189		40.89	C
MOTA	4124	CG	ASN		3	75.927		204.587		45.78	C
ATOM	4125		ASN		3	77.027		204.237		50.88	C
MOTA	4126		ASN		3	75.765		205.313		47.22	C
MOTA	4127	C	ASN	C 6	3	72.874	85.778	202.587	1.00	37.28	C

MOTA	4128	0	ASN	Ċ 6	3	72.804	86.594	201.661	1.00	39.40	С
ATOM	4129	N	THR	C 6	4	71.885	85.525	203.435	1.00	33.11	· c
MOTA	4130	CA	THR	C 6	4	70.604	86.177	203.283	1.00	34.48	C
MOTA	4131	CB	THR	C 6	4	69.497	85.156	203.035	1.00	32.27	C
ATOM	4132	OG1	THR	C 6	4	69.873	84.305	201.948	1.00	44.70	C
MOTA	4133	CG2	THR	C 6	4	68.197	85.864	202.693	1.00	30.86	C
MOTA	4134	C	THR	C 6	4	70.163		204.442		36.22	C
ATOM	4135	Ō	THR			70.185		205.599		40.90	Ċ
ATOM	4136	N	LEU			69.754		204.112		36.10	Č
ATOM	4137	CA	LEU			69.246		205.099		37.30	Č
ATOM	4138	CB	LEU			69.646		204.738		32.48	č
ATOM	4139	CG	LEU			71.131		204.855		30.07	Č
ATOM	4140		LEU			71.394		204.544		31.04	Č
ATOM	4141	CD2				71.592		206.250		36.01	Ċ
ATOM	4142	C	LEU			67.728		205.050		39.45	č
ATOM	4143	Ō	LEU			67.158		203.968		35.94	Ċ
ATOM	4144	N	ARG			67.083		206.215		41.50	Ċ
ATOM	4145	CA	ARG			65.629		206.289	•	42.71	Ċ
ATOM	4146	CB	ARG			65.232		207.083		42.21	Č
ATOM	4147	CG	ARG			65.753		206.491		50.83	Č
ATOM	4148	CD	ARG			65.505		207.415		58.84	č
ATOM	4149	NE	ARG			66.419		207.135		59.81	Č
ATOM	4150	CZ	ARG			66.389		206.031		59.51	Č
ATOM	4151	NH1				65.483		205.098		61.29	č
ATOM	4152	NH2				67.272		205.854		65.54	Ċ
ATOM	4153	C	ARG			65.074		206.965		43.68	č
ATOM	4154	ō	ARG			65.483		208.080		47.33	č
ATOM	4155	N	ILE			64.163		206.279		40.46	Ċ
ATOM	4156	CA	ILE			63.554		206.805		39.13	č
ATOM	4157	CB	ILE			63.305		205.702		37.41	č
ATOM	4158	CG2	ILE			62.526		206.266		40.71	Č
ATOM	4159	CG1				64.627		205.128		39.69	Ċ
ATOM	4160		ILE			65.271		204.149		42.41	Č
ATOM	4161	C .	ILE			62.218		207.476		42.16	Ċ
ATOM	4162	0	ILE			61.262		206.843		41.63	Č
ATOM	4163	N	LEU			62.143		208.762		39.83	č
ATOM	4164	CA	LEU			60.935		209.513		39.35	Č
ATOM	4165	CB	LEU			61.281		210.846		38.99	Ċ
ATOM	4166	CG	LEU			62.266		210.825		33.23	Ċ
ATOM	4167		LEU			62.496		212.246		32.97	C
ATOM	4168		LEU			61.728		209.990		38.69	Ċ
ATOM	4169	C	LEU			60.104		209.780		42.26	C
ATOM	4170	Ō	LEU			60.622	· -	210.161		40.16	Č
MOTA	4171	N	ASP			58.799		209.600		44.01	Ċ
ATOM	4172	CA	ASP			57.809		209.809		43.20	C
MOTA	4173	CB	ASP			56.539		209.082		41.80	č
MOTA	4174	CG	ASP			55.394		209.298		47.86	Ċ
ATOM	4175		ASP			54.324		208.682		53.00	c
MOTA	4176		ASP			55.551		210.074		37.17	, c
ATOM	4177	C	ASP			57.546		211.302		47.45	Ċ
ATOM	4178	0	ASP			56.994		211.941		50.90	C
ATOM	4179	N	ALA			57.959		211.872		52.18	č
ATOM	4180	CA	ALA			57.719		213.288		61.22	č
ATOM	4181	CB	ALA			58.917		213.230		61.48	Ċ
ATOM	4182	c	ALA			56.508		213.403		69.44	Č
ATOM	4183	ō	ALA			55.789		214.401		72.24	č
MOTA	4184	N	THR			56.291		212.361		78.15	Č
MOTA	4185	CA	THR			55.172		212.324		84.88	c
				•							-

MOTA	4186	CB	THR	C	71	55.250	99.043	211.090	1.00 82.25	C
MOTA	4187	OG1	THR	C	71	54.069	99.849	211.037	1.00 83.66	C
ATOM	4188	CG2	THR	С	71	55.378	98.260	209.796	1.00 82.08	C
MOTA	4189	Ç	THR	C	71	53.848	97.347	212.303	1.00 91.28	С
MOTA	4190	0	THR	C	71	53.427	96.826	211.262	1.00 93.29	C
MOTA	4191	N	ASN	C	72	53.203	97.290	213.466	1.00 95.44	C
MOTA	4192	CA	ASN	C	72	51.920	96.610	213.600	1.00 99.89	C
ATOM	4193	CB	ASN	C	72	51.500	96.567	215.076	1.00105.66	C
MOTA	4194	CG	ASN	C	72	52.211	95.472	215.860	1.00110.37	C
MOTA	4195	OD1	ASN	C	72	51.986	95.309	217.063	1.00110.22	C
ATOM	4196	ND2	ASN	C	72	53.070	94.710	215.179	1.00112.45	C
MOTA	4197	С	ASN	C	72	50.833	97.299	212.771	1.00100.19	C
MOTA	4198	0	ASN	C	72	49.906	97.900	213.320	1.00101.88	С
MOTA	4199	N	ASN	C	73	50.953	97.211	211.449	1.00 98.55	С
MOTA	4200	CA	ASN	C	73	49.984	97.824	210.545	1.00 95.87	. C
ATOM	4201	CB	ASN	C	73	48.715	96.965	210.472	1.00 98.58	C
MOTA	4202	CG	ASN	C	73	49.013	95.477	210.405	1.00101.36	C
MOTA	4203	OD1	ASN	C	73	49.550	94.891	211.351	1.00101.49	C
ATOM	4204	ND2	ASN	C	73	48.662	94.856	209.286	1.00100.77	C
MOTA	4205	C	ASN	С	73	49.616	99.234	211.024	1.00 92.07	C
ATOM	4206	0	ASN	C	73	48.463	99.652	210.920	1.00 91.51	C
MOTA	4207	N	GLN	С	74	50.598	99.956	211.560	1.00 86.79	С
ATOM	4208	CA	GLN	C	74	50.375	101.312	212.057	1.00 81.00	C
ATOM	4209	CB	GLN	C	74	51.242	101.557	213.301	1.00 86.33	C
MOTA	4210	CG	GLN	C	74	50.917	100.604	214.467	1.00 92.89	C
ATOM	4211	CD	GLN	C	74	51.999	100.545	215.552	1.00 94.78	Ċ
MOTA	4212	OE1	GLN	C	74	51.852	99.830	216.549	1.00 91.99	C
MOTA	4213	NE2	GLN	С	74	53.087	101.288	215.356	1.00 94.14	С
ATOM	4214	C	GLN	C	74	50.700	102.335	210.973	1.00 74.13	C
MOTA	4215	0 -	GLN	C	74	50.798	103.534	211.241	1.00 72.76	C
MOTA	4216	N	LEU	C	75	50.859	101.846	209.746	1.00 66.10	C
ATOM	4217	CA	LEU	C	75	51.174	102.696	208.601	1.00 60.39	C
MOTA	4218	CB	LEU	C	75	52.283	102.062	207.752	1.00 49.63	C
MOTA	4219	CG	LEU	C	75	53.652	101.815	208.376	1.00 46.54	С
MOTA	4220	CD1	LEU	С	75	54.421	100.847	207.509	1.00 42.39	С
MOTA	4221	CD2	LEU	C	75	54.403	103.119	208.541	1.00 36.34	С
ATOM	4222	C	LEU	С	75	49.956	102.896	207.709	1.00 60.12	C
MOTA	4223	0	LEU	C	75	49.005	102.118	207.748	1.00 62.73	С
ATOM	4224	N	PRO	С	76		103.950		1.00 58.03	C
MOTA	4225	CD	PRO	C	76	50.983	105.014	206.807	1.00 58.07	C
MOTA	4226	CA	PRO	C	76	48.856	104.224	205.981	1.00 59.78	C
ATOM	4227	CB	PRO	С	76	49.387	105.381	205.143	1.00 55.14	C
ATOM	4228	CG	PRO	C	76	50.222	106.117	206.112	1.00 53.65	C
MOTA	4229	С	PRO	С	76	48.579	102.974	205.134	1.00 62.32	C
MOTA	4230	0	PRO	C	76	49.515	102.318	204.681	1.00 62.07	С
MOTA	4231	N	GLN	C	77				1.00 64.58	С
MOTA	4232	CA	GLN	С	77	46.952	101.464	204.137	1.00 64.79	С
ATOM	4233	CB	GLN	С	77	45.908	100.647	204.891	1.00 64.74	C
MOTA	4234	CG	GLN	C	77	46.429	100.094	206.195	1.00 69.48	C
MOTA	4235	CD	GLN	С	77	47.682		206.002	1.00 72.27	C
MOTA	4236		GLN		77	48.673		206.716	1.00 72.62	C
MOTA	4237	NE2	GLN		77		98.361		1.00 72.12	C
MOTA	4238	C	GLN		77			202.708	1.00 63.22	С
MOTA	4239	0	GLN		77			201.986	1.00 62.43	C
MOTA	4240	N	ASP		78			202.298	1.00 61.10	C
MOTA	4241	CA	ASP	C	78	46.018	103.333	200.954	1.00 59.37	C
MOTA	4242	CB	ASP		78 .			201.003	1.00 59.11	C
MOTA	4243	CG	ASP	С	78	45.806	105.758	201.668	1.00 63.32	C

MOTA	4244	OD1	ASP C	78	45.328 106.895 201.486 1.00 65.	38 C
MOTA	4245	OD2	ASP C	78	46.810 105.560 202.379 1.00 68.	55 C
ATOM	4246	C	ASP C	78	47.184 103.589 199.999 1.00 60.	48 C
MOTA	4247	0	ASP C	78	47.009 103.621 198.781 1.00 62.	
ATOM	4248	N	ARG C		48.380 103.753 200.548 1.00 60.	
ATOM	4249	CA	ARG C		49.550 104.050 199.734 1.00 55.	
ATOM	4250	CB	ARG C			
ATOM	4251	CG	ARG C		50.082 106.127 201.084 1.00 55.	
MOTA	4252	CD	ARG C	79	49.861 107.613 201.134 1.00 53.	84 C
ATOM	4253	NE	ARG C	79	48.436 107.893 201.074 1.00 59.	74 C
MOTA	4254	cz	ARG C	79	47.911 109.095 200.873 1.00 61.	98 C
MOTA	4255	NH1	ARG C	79	48.695 110.155 200.708 1.00 60.	
ATOM	4256	NH2	ARG C	79	46.594 109.227 200.825 1.00 61.	
ATOM	4257	C	ARG C		50.780 103.393 200.316 1.00 50.	
ATOM	4258	ō	ARG C		50.743 102.891 201.437 1.00 50.	
		И	GLU C			
ATOM	4259				51.870 103.405 199.557 1.00 45.	
ATOM	4260	CA	GLU C		53.119 102.825 200.032 1.00 41.	
MOTA	4261	CB	GLU C		54.104 102.601 198.894 1.00 39.	
ATOM	4262	CG	GLU C	80	53.633 101.772 197.733 1.00 37.	34 C
MOTA	4263	· CD	GLU C	80	54.725 101.628 196.689 1.00 36.	26 C
ATOM	4264	OE1	GLU C	80	55.218 100.501 196.481 1.00 29.	36 C
MOTA	4265	OE2	GLU C	80	55.103 102.655 196.084 1.00 39.	
ATOM	4266	C	GLU C	80	53.755 103.836 200.972 1.00 42.	
ATOM	4267	Ō	GLU C		53.494 105.037 200.879 1.00 43.	
ATOM	4268	И	SER C		54.587 103.350 201.883 1.00 41.	
ATOM	4269	CA	SER C			
MOTA	4270	CB	SER C		54.998 103.849 204.243 1.00 38.	
ATOM	4271	OG	SER C		53.618 103.999 204.537 1.00 46.	
MOTA	4272·	С	SER C		56.760 104.051 202.461 1.00 39.	
ATOM	4273	0	SER C	81	57.229 102.922 202.291 1.00 42.	
ATOM	4274	N	LEU C	82	57.484 105.160 202.336 1.00 37.	81 C
ATOM	4275	CA	LEU C	82	58.907 105.107 202.005 1.00 37.	17 C
MOTA	4276	CB	LEU C	82	59.327 106.400 201.309 1.00 35.	
MOTA	4277	CG	LEU C	82	60.825 106.670 201.142 1.00 37.	
ATOM	4278		LEU C	82	61.555 105.491 200.547 1.00 27.	
ATOM	4279		LEU C	82	60.980 107.880 200.265 1.00 38.	
ATOM	4280	C	LEU C	82	59.819 104.858 203.198 1.00 36.	
ATOM			LEU C			
	4281	0			59.673 105.494 204.247 1.00 34.	
ATOM	4282	N	PHE C		60.753 103.923 203.022 1.00 34.	
ATOM	4283	CA	PHE C		61.733 103.583 204.053 1.00 34.	
MOTA	4284	CB	PHE C		61.344 102.308 204.788 1.00 32.	
ATOM	4285	CG	PHE C	83	60.221 102.491 205.751 1.00 39.	
ATOM	4286	CD1	PHE C	83	58.901 102.540 205.310 1.00 32.	49 C
MOTA	4287	CD2	PHE C	83	60.484 102.652 207.110 1.00 42.	10 C
ATOM	4288	CE1	PHE C	83	57.869 102.743 206.204 1.00 30.	
MOTA	4289	CE2	PHE C	83	59.453 102.856 208.012 1.00 35.	
ATOM	4290	CZ	PHE C		58.145 102.901 207.552 1.00 40.	
ATOM	4291	C	PHE C		63.096 103.382 203.411 1.00 34.	
ATOM	4292	ō	PHE C			
MOTA	4293	N	TRP C		64.141 103.367 204.229 1.00 32.	
MOTA	4294	CA	TRP C		65.468 103.170 203.702 1.00 26.	
MOTA	4295	CB	TRP C		66.264 104.457 203.781 1.00 17.	
MOTA	4296	CG	TRP C		65.695 105.511 202.912 1.00 21.	
MOTA	4297	CD2			66.001 105.753 201.528 1.00 16.	
MOTA	4298	CE2	TRP C	84	65.224 106.854 201.116 1.00 16.	
MOTA	4299	CE3	TRP C	84	66.849 105.140 200.597 1.00 22.	
MOTA	4300		TRP C		64.770 106.443 203.266 1.00 21.	21 C
ATOM	4301		TRP C		64.486 107.261 202.196 1.00 23.	

ATOM	4302		TRP	C	84	65.269	107.360	199.813	1.00	18.40	C
MOTA	4303	CZ3	TRP	С	84	66.895	105.646	199.296	1.00	12.77	C
ATOM	4304	CH2	TRP	C	84	66.111	106.742	198.922	1.00	17.00	C
MOTA	4305	С	TRP	C	84	66.209	102.051	204.385	1.00	29.58	C
MOTA	4306	0	TRP	С	84	66.373	102.045	205.601	1.00	33.29	C
MOTA	4307	N	MET	C	85	66.651	101.107	203.561	1.00	30.91	C
MOTA	4308	CA	MET	С	85	67.382	99.917	203.962	1.00	27.89	С
ATOM	4309	CB	MET	C	85	66.965	98.776	203.028	1.00	27.01	C
MOTA	4310	CG	MET	С	85	67.759	97.494	203.151	1.00	33.69	C
ATOM	4311	SD	MET	С	85	67.324	96.526	204.573	1.00	40.67	C
ATOM	4312	CE	MET	C	85	68.475	95.159	204.440		31.35	C
MOTA	4313	C	MET	C	85	68.887	100.202	203.863	1.00	28.56	C
ATOM	4314	0	MET	С	85	69.380	100.659	202.820	1.00	27.79	C
MOTA	4315	N	ASN	C	86	69.608	99.942	204.954	1.00	27.95	С
ATOM	4316	CA	ASN	C ·	86	71.054	100.183	205.010	1.00	25.57	С
MOTA	4317	CB	ASN	С	86	71.393	101.320	206.001	1.00	19.17	C
MOTA	4318	CG	ASN	С	86	70.826	102.676	205.571	1.00	26.85	C
MOTA	4319	OD1	ASN	С	86	69.643	102.963	205.778	1.00	29.10	C
ATOM	4320	ND2	ASN	C	86	71.668	103.512	204.971	1.00	21.29	С
ATOM	4321	C	ASN	C	86	71.816	98.932	205.410	1.00	24.24	С
MOTA	4322	0	ASN	С	86	71.456	98.272	206.367	1.00	28.42	С
MOTA	4323	N	VAL	C	87	72.870	98.613	204.661	1.00	26.20	C
MOTA	4324	CA	VAL	G.	87	73.709	97.447	204.923	1.00	21.04	С
MOTA	4325	CB	VAL	С	87	73.517	96.362	203.840	1.00	20.01	C
MOTA	4326	·CG1	VAL	С	87	74.441	95.169	204.094	1.00	11.59	C
MOTA	4327		VAL		87	72.053	95.910	203.820	1.00	10.62	C
MOTA	4328	C	VAL	С	87	75.139	97.968	204.897	1.00	27.14	С
ATOM	4329	0	VAL	C	87	75.655	98.412	203.862	1.00	26.21	C
MOTA	4330	N	LYS	С	88	75.745	97.932	206.075	1.00	29.25	C
ATOM	4331	CA	LYS	С	88	77.094	98.406	206.312	1.00	30.45	C
MOTA	4332	CB	LYS	C	88	77.112	99.136	207.645	1.00	26.10	C
ATOM	4333	CG	LYS	C	88	78.440	99.610	208.120	1.00	27.13	С
MOTA	4334	CD	LYS	С	88	78.204	100.714	209.123	1.00	30.18	C
ATOM	4335	CE	LYS	C	88	79.384	100.916	210.032	1.00	34.56	C
MOTA	4336	NZ	LYS	C	88	78.971	101.839	211.098	1.00	33.72	С
MOTA	4337	C	LYS	C	88	78.094	97.272	206.332	1.00	31.26	C
MOTA	4338	0	LYS	С	88	77.827	96.224	206.904	1.00	35.75	C
ATOM	4339	N	ALA	С	89	79.244	97.480	205.701	1.00	32.14	C
ATOM	4340	CA	ALA	С	89	80.280	96.462	205.681	1.00	35.00	С
MOTA	4341	CB	ALA		89	80.755	96.228	204.267	1.00	38.93	C
MOTA	4342	C	ALA	С	89	81.436	96.934	206.553	1.00	36.63	C
ATOM	4343	0	ALA	С	89	82.222	97.786	206.157	1.00	38.46	С
MOTA	4344	N	ILE	C	90	81.532	96.374	207.748	1.00	38.33	C
MOTA	4345	CA	ILE	C	90	82.583	96.747	208.680	1.00	44.39	С
MOTA	4346	CB	ILE	С	90	82.106	96.567	210.139	1.00	43.19	С
MOTA	4347		ILE	-	90	83.239		211.090		38.20	С
MOTA	4348		ILE		90	80.894		210.408		43.19	C
MOTA	4349	CD1	ILE	C	90	80.269		211.767	1.00	38.45	С
MOTA	4350	C	ILE		90	83.861	95.928	208.494		50.06	C
MOTA	4351	0	ILE		90	83.863		208.626		51.70	C
MOTA	4352	N	PRO		91	84.972	96.601	208.181		51.91	С
MOTA	4353	CD	PRO		91	85.174		207.845		50.07	C
ATOM	4354	CA	PRO		91	86.207		208.008		54.21	C
ATOM	4355	CB	PRO		91	87.122		207.320	1.00	48.24	C
MOTA	4356	CG	PRO		91	86.682		207.894		51.18	C
MOTA	4357	С	PRO		91	86.719		209.372	1.00	58.98	C
MOTA	4358	0	PRO	С	91	85.942		210.294		58.55	C
ATOM	4359	N	SER	С	92	88.029	95.249	209.497	1.00	66.08	C

MOTA	4360	CA	SER	C	92	88.634	94.815	210.745	1.00 67.26	.C
MOTA	4361	CB	SER	C	92	88.958		210.648	1.00 66.19	C
MOTA	4362	OG	SER	C	92	89.323	92.991	209.315	1.00 67.25	C
MOTA	4363	C	SER	C	92	89.890	95.636	210.954	1.00 70.18	C
MOTA	4364	0	SER	C	92	90.514		209.985	1.00 72.54	C
MOTA	4365	N	MET	С	93	90.260	95.881	212.207	1.00 75.94	C
MOTA	4366	CA	MET	C	93	91.450		212.515	1.00 81.70	C
MOTA	4367	CB	MET	C	93	91.393	97.175	213.970	1.00 88.65	С
MOTA	4368	CG	MET	С	93	92.345	98.340	214.300	1.00 98.39	C
MOTA	4369	SD	MET	C	93	94.051	97.929	214.834	1.00105.77	C
MOTA	4370	CE	MET	C	93	94.070	98.632	216.490	1.00100.27	C
MOTA	4371	С	MET	C	93	92.754	95.916	212.292	1.00 82.57	C
MOTA	4372	0	MET	C	93	92.954	94.842	212.863	1.00 80.96	C
ATOM	4373	N	ASP	C	94	93.629	96.471	211.451	1.00 84.66	C
ATOM	4374	CA	ASP	C	94	94.923	95.850	211.184	1.00 86.49	C
MOTA	4375	CB	ASP	С	94	95.664	96.511	210.009	1.00 87.53	C
MOTA	4376	CG	ASP	C	94	94.902	96.440	208.697	1.00 92.41	C
MOTA	4377	OD1	ASP	C	94	95.563		207.631	1.00 87.30	C
MOTA	4378	OD2	ASP	C	94	93.652		208.726	1.00 94.22	C
ATOM	4379	C	ASP	C	94	95.768	96.062	212.422	1.00 87.82	C
ATOM	4380	0	ASP		94	95.988		212.834	1.00 88.63	C
MOTA	4381	N	LYS	C	95	96.230	94.978	213.030	1.00 88.84	C
MOTA	4382	CA	LYS	С	95	97.086	95.105	214.197	1.00 88.45	C
MOTA	4383	CB	LYS	C	95	97.128	93.790	214.972	1.00 87.51	C
MOTA	4384	CG	LYS	C	95	95.839	93.461	215.706	1.00 85.60	C
MOTA	4385	CD	LYS	C	95	94.725	93.020	214.781	1.00 88.20	C -
ATOM	4386	CE	LYS	С	95	94.966	91.618	214.234	1.00 88.04	C
MOTA	4387	NZ	LYS		95	93.794		213.462	1.00 85.88	C
MOTA	4388	C	LYS		95	98.457	95.434	213.620	1.00 89.08	C
ATOM	4389.	0	LYS		95	99.438		214.340	1.00 88.70	C
MOTA	4390	N	SER		96	98.485		212.295	1.00 91.18	C
MOTA	4391	CA	SER		96	99.688		211.527	1.00 91.60	C
MOTA	4392	CB	SER		96	99.590		210.154	1.00 92.40	C
MOTA	4393	OG	SER		96	98.391		209.483	1.00 90.75	C
MOTA	4394	C	SER		96	99.984		211.334	1.00 91.57	C
MOTA	4395	0	SER		96	101.149		211.290	1.00 92.99	C
MOTA	4396	N	LYS		97	98.941	98.153		1.00 89.94	C
ATOM	4397	CA	LYS		97	99.130		211.008	1.00 89.77	C
MOTA	4398	CB	LYS		97		100.095		1.00 91.96	C
ATOM	4399	CG	LYS		97	98.266		208.601	1.00 96.47	. C
ATOM	4400	CD	LYS		97	99.650		207.984	1.00101.18	C
MOTA	4401	CE	LYS		97	99.629		206.757	1.00102.44	C
ATOM	4402	NZ	LYS		97	100.994		206.207	1.00104.46	C
MOTA		. G	LYS		97		100.337		1.00 87.93	C
ATOM	4404	0.	LYS		97		101.552		1.00 88.12	C
MOTA	4405	N	LEU		98	98.711		213.377	1.00 87.66	C
ATOM	4406 4407	CA	LEU		98		100.096		1.00 88.51	C
MOTA		CB	LEU		98	98.568		215.721	1.00 90.90	C
MOTA MOTA	4408 4409	CG	LEU		98	98.300 99.507		217.215	1.00 92.39	C
					98				1.00 90.36	C
MOTA MOTA	4410 4411	CD2 C	LEU		98 98		100.006		1.00 93.94	C
	4411		FEA						1.00 87.33	C
ATOM	4412	O N			98		102.272		1.00 86.68	C
ATOM	4413	N	THR		99				1.00 85.49	C
MOTA MOTA	4414	CA	THR		99		102.667 102.302		1.00 81.70	C
ATOM	4415	CB	THR THR		99		102.302		1.00 83.64 1.00 84.13	C
ATOM	4417	CG2			99 99		101.821			C C
WI OLI	-T-T-1	CG2	TUK	C	フフ	T07.433	TOT.53T	~ × 1 . U > O	1.00 80.79	C

		_							
ATOM	4418	С	THR C			103.606		1.00 79.48	С
ATOM	4419	0	THR C	99	102.323	104.330	214.143	1.00 77.78	С
ATOM	4420	N	GLU C	100	100.370	103.578	213.318	1.00 78.70	С
ATOM	4421	CA	GLU C	100	100.408	104.413	212.132	1.00 76.77	C
ATOM	4422	CB	GLU C	100	100.483	103.542	210.880	1.00 79.30	С
ATOM	4423	CG	GLU C			102.911		1.00 84.62	Č
ATOM	4424	CD	GLU C			101.911		1.00 85.94	Ċ
ATOM			GLU C						
	4425					102.263		1.00 88.43	C
ATOM	4426	OE2				100.772		1.00 88.44	С
MOTA	4427	C	GLU C			105.305		1.00 73.28	C
ATOM	4428	0	GLU C	100	98.172	105.067	212.676	1.00 72.87	C
ATOM	4429	N	ASN C	101	99.304	106.342	211.209	1.00 70.85	C
ATOM	4430	CA	ASN C	101	98.199	107.250	210.971	1.00 68.56	C
ATOM	4431	CB	ASN C	101	98.721	108.602	210.512	1.00 68.80	C
ATOM	4432	CG	ASN C			109.561		1.00 74.73	Ċ
ATOM	4433	_	ASN C			109.144		1.00 74.69	Ċ
ATOM	4434		ASN C			110.855			C
								1.00 77.18	
ATOM	4435	C	ASN C			106.583		1.00 66.16	C
ATOM	4436	0	ASN C			106.436		1.00 65.12	C
ATOM	4437	N	THR C			106.171		1.00 62.42	С
MOTA	4438	CA	THR C	102	95.347	105.470	209.240	1.00 60.02	С
ATOM	4439	CB	THR C	102	95.221	103.995	209.626	1.00 61.43	С
MOTA	4440	OG1	THR C	102	94.630	103.897	210.926	1.00 65.81	C
ATOM	4441	CG2	THR C	102	96.590	103.336	209.658	1.00 67.01	C
MOTA	4442	C	THR C			106.000		1.00 55.44	Ċ
ATOM	4443	ō	THR C			106.748		1.00 49.92	Ċ
ATOM	4444	N	LEU C			105.607		1.00 54.74	č
ATOM		CA	LEU C			105.007			c
	4445							1.00 53.90	
MOTA		CB	LEU C			107.010		1.00 49.57	C
ATOM .	4447	CG	TEA C			107.181		1.00 50.56	С
MOTA	4448		LEU C		89.617	107.820	207.034	1.00 49.66	C
MOTA	4449	CD2	PEA C		90.435	108.027	204.680	1.00 49.68	C
ATOM	4450	С	LEU C	103	91.287	104.724	207.069	1.00 50.03	C
MOTA	4451	0	LEU C	103	91.750	104.053	206.150	1.00 46.64	С
MOTA	4452	N	GLN C	104	90.173	104.398	207.703	1.00 49.55	С
ATOM	4453	CA	GLN C	104	89.421	103.243	207.260	1.00 50.66	c.c
ATOM	4454	CB	GLN C			102.193		1.00 50.09	Č
ATOM	4455	CG	GLN C			100.949		1.00 47.02	č
ATOM	4456	CD	GLN C		89.953		209.050	1.00 44.86	c
ATOM	4457		GLN C		90.494		208.882	1.00 44.24	C
ATOM	4458		GLN C			100.115		1.00 43.43	C
MOTA	4459	C	GLN C			103.655		1.00 47.86	С
MOTA	4460	0	GLN C			104.538		1.00 45.75	C
ATOM	4461	N	LEU C	105	87.590	103.031	205.714	1.00 41.37	С
ATOM	4462	CA	LEU C	105	86.279	103.327	205.198	1.00 39.67	С
MOTA	4463	CB	LEU C	105	86.339	103.572	203.699	1.00 41.36	C
ATOM	4464	CG	LEU C	105	87.166	104.767	203.233	1.00 40.66	C
MOTA	4465		LEU C			104.929		1.00 45.24	Ċ
ATOM	4466		LEU C			106.027		1.00 44.36	Ċ
ATOM	4467	C	LEU C			102.148		1.00 38.36	č
ATOM	4468	0	LEU C			101.023		1.00 40.09	c
ATOM	4469	N	ALA C			102.429		1.00 35.79	C
ATOM	4470	CA	ALA C			101.413		1.00 28.97	C
MOTA	4471	CB	ALA C			101.562		1.00 29.44	С
MOTA	4472	C	ALA C			101.690		1.00 28.76	C
ATOM	4473	0	ALA C	106		102.704		1.00 32.17	Ċ
MOTA	4474	N	ILE C	107	81.951	100.808	203.785	1.00 26.90	C
ATOM	4475	CA	ILE C			100.995		1.00 24.23	Ċ
							· - · -		

ATOM	4476	CB	ILE C	107	81.373	100.155	201.487	1.00 24.81	C
MOTA	4477	CG2	ILE C	107	80.588	100.645	200.257	1.00 23.07	C
ATOM	4478	CG1				100.284		1.00 21.30	C
MOTA	4479	CD1				101.668		1.00 20.95	C
ATOM	4480	C	ILE C		79.625	100.573	203.178	1.00 26.48	C
MOTA	4481	0	IFE C		79.483		203.907	1.00 29.41	С
MOTA	4482	N	ILE C			101.322		1.00 25.57	C
ATOM	4483	CA	ILE C			101.015		1.00 29.03	C
MOTA	4484	CB	ILE C			102.055		1.00 31.74	C
ATOM	4485	CG2	ILE C		75.282		204.577	1.00 23.26	C
ATOM	4486	CG1	ILE C			102.210		1.00 27.10	C
ATOM	4487	CD1	ILE C			103.432		1.00 20.06	C
ATOM	4488	C	ILE C			101.083		1.00 28.55	C
ATOM	4489	0	ILE C SER C			101.924		1.00 27.49	C
ATOM ATOM	4490 4491	N CA	SER C			100.193 100.238		1.00 27.78	C
ATOM	4491	CB	SER C		74.514		199.939	1.00 29.78 1.00 29.22	C
ATOM	4493	OG	SER C		75.687		199.544	1.00 29.22	C
ATOM	4494	C	SER C			100.657		1.00 30.92	· C
ATOM	4495	ō	SER C			100.037		1.00 31.20	C
ATOM	4496	N	ARG C			101.700		1.00 25.46	C
ATOM	4497	CA	ARG C			102.210		1.00 28.53	Ċ
MOTA	4498	СВ	ARG C			;103.649		1.00 23.33	Č
ATOM	4499	CG	ARG C			:104.509		1.00 27.53	Č
ATOM	4500	CD	ARG C			.105.913		1.00 23.03	Č
ATOM	4501	NE	ARG C			105.822		1.00 32.98	Č
ATOM	4502	CZ	ARG C	110	69.476	106.416	204.357	1.00 31.72	C
ATOM	4503	NH1	ARG C	110	68.490	107.186	203.914	1.00 20.17	C
ATOM	4504	NH2			69.601	106.191	205.654	1.00 27.52	C
MOTA	4505	C	ARG C	110	70.305	102.195	200.024	1.00 34.31	C
MOTA	4506	0	ARG C	110	70.468	102.909	199.028	1.00 33.63	С
MOTA	4507	N	ILE C		69.258	101.389	200.181	1.00 35.76	C
MOTA	4508	CA	ILE C	111	68.241	101.269	199.158	1.00 29.74	C
MOTA	4509	CB	ILE C		68.312	99.895	198.520	1.00 30.13	C
MOTA	4510	CG2			69.689	99.711	197.867	1.00 30.10	C
ATOM	4511	CG1	ILE C		68.060		199.581	1.00 27.37	C
MOTA	4512		ILE C		67.937		199.020	1.00 26.04	C
MOTA	4513	C	ILE C			101.504		1.00 25.68	C
MOTA	4514	0	ILE C			101.342		1.00 25.24	C
MOTA	4515	N	LYS C			101.879		1.00 23.97	C
ATOM	4516	CA	LYS C			102.132		1.00 27.13	C
MOTA	4517	CB	LYS C			102.802		1.00 23.28	C
MOTA	4518	CG	LYS C			103.936		1.00 24.02	C
ATOM ATOM	4519 4520	CD	LYS C			104.395		1.00 34.80 1.00 44.00	C
ATOM	4521	NZ	LYS C			105.466 105.871		1.00 44.00	c
ATOM	4521	C	LYS C			100.827		1.00 46.30	C
ATOM	4523	0	LYS C		64.128		198.965	1.00 26.75	C
ATOM	4524	N	LEU C			100,921		1.00 26.13	c
MOTA	4525	CA.	LEU C		62.186		200.911	1.00 29.40	c
MOTA	4526	CB	TEO C		62.617		202.305	1.00 27.31	Ċ
MOTA	4527	CG	LEU C		61.661		202.305	1.00 27.04	c
ATOM	4528		TEA C		61.033		202.099	1.00 42.12	Ċ
ATOM	4529		LEU C		62.431		204.118	1.00 29.99	Ċ
ATOM	4530	C	LEU C			100.333		1.00 33.39	Ċ,
MOTA	4531	ŏ	LEU C			101.282		1.00 40.52	č.
ATOM	4532	N	TYR C		59.880		200.122	1.00 29.57	č
MOTA	4533	CA	TYR C			100.273		1.00 32.86	Ċ

MOTA	4534	CB	TYR	C	114	57.930	100.481	198.748	1.00	30.74	С
MOTA	4535	CG	TYR		114	58.650	101.478	197.892	1.00	29.60	C
MOTA	4536	CD1	TYR	С	114	59.406	101.062	196.802	1.00	26.10	C
ATOM	4537	CE1	TYR	C	114	60.068	101.969	196.014	1.00	23.29	C
MOTA	4538	CD2	TYR		114	58.574	102.838	198.163	1.00	29.47	С
MOTA	4539	CE2	TYR	C	114	59.235	103.761	197.368	1.00	26.92	С
MOTA	4540	CZ	TYR	С	114	59.979	103.319	196.299	1.00	26.65	C
ATOM	4541	OH	TYR				104.224	195.506	1.00	33.22	C
ATOM	4542	С	TYR	C	114	57.605	99.298	200.880	1.00	34.84	C
MOTA	4543	0	TYR	C	114	57.677		200.679	1.00	34.64	C
MOTA	4544	N	TYR			56.765		201.743		35.45	C
MOTA	4545	CA	TYR	C	115	55.786	99.056	202.463	1.00	39.69	C
MOTA	4546	CB	TYR			55.482	99.703	203.815	1.00	41.42	C
ATOM	4547	CG	TYR			54.400		204.590		45.34	C
ATOM	4548		TYR			54.647		205.211	1.00	47.77	C
ATOM	4549		TYR			53.655		205.925		48.10	C
MOTA	4550	CD2	TYR			53.120		204.699	1.00	46.27	C
ATOM	4551		TYR			52.117		205.412		47.07	C
MOTA	4552	CZ	TYR			52.393		206.023		48.41	C
ATOM	4553	OH	TYR			51.416		206.733		53.80	C
ATOM	4554	C	TYR	-		54.593		201.524		41.45	C
ATOM	4555	0	TYR				100.313			42.19	C
ATOM	4556	N	ARG			54.205		200.841		46.96	C
MOTA	4557	CA	ARG		116	53.091		199.906		48.56	С
ATOM	4558	CB	ARG			53.478		198.582		50.98	C
ATOM	4559	CG	ARG			52.379		197.515		56.25	C
ATOM	4560	CD	ARG			52.923		196.160		51.16	C
ATOM	4561	NE	ARG			53.861		195.633		53.13	C
MOTA	4562	CZ	ARG			54.795		194.726		48.89	C
MOTA	4563		ARG			54.912		194.248		46.77	C
ATOM	4564		ARG			55.612		194.300		46.98	C
	4565	C	ARG			51.832		200.447		51.42	C
ATOM	4566	0	ARG			51.708		200.453		54.30	C
ATOM	4567	N	PRO			50.879		200.917		56.53	C
ATOM	4568	CD	PRO			50.852		200.908		58.77	C
MOTA	4569	CA	PRO PRO			49.627		201.456		62.45	C
MOTA MOTA	4570	CB CG	PRO			48.755	100.174	201.625		60.03	C C
ATOM	4571 4572	C	PRO			49.747		201.692		58.16 66.70	c
ATOM	4573	0	PRO			48.544		199.406		69.54	C
ATOM	4574	N	ALA			49.134		200.703		73.31	c
ATOM	4575	CA	ALA			48.602		199.776		79.41	· c
MOTA	4576	CB	ALA			49.093		200.164		83.73	c
MOTA	4577	C	ALA			47.076		199.811		80.96	C
ATOM	4578	o	ALA			46.447		200.628		82.02	· c
ATOM	4579	N	LYS			46.494		198.928		81.32	ď
ATOM	4580	CA	LYS			45.041		198.853		80.16	Č
ATOM	4581	CB	LYS			44.473		200.257		80.43	Č
ATOM	4582	CG	LYS			42.987		200.409		82.71	č
ATOM	4583	CD	LYS			42.715		200.551		81.14	Č
ATOM	4584	CE	LYS			41.288		201.047		84.48	č
ATOM	4585	NZ	LYS			40.998		201.358		83.97	Č
ATOM	4586	C	LYS			44.686		197.974		79.67	Č
ATOM	4587	ō	LYS			43.573		198.043		79.79	č
ATOM	4588	N	LEU			45.630		197.144		78.27	Č
ATOM	4589	CA	LEU			45.413		196.280		77.14	
ATOM	4590	CB	LEU			46.727		196.103		77.38	C
ATOM	4591	CG	LEU			47.530		197.393		76.41	С

MOTA	4592	CD1	LEU	С	120	48.829	100.148	197.083	1.00	75.66	C
MOTA	4593	CD2	LEU	С	120	46.705	100.200	198.407	1.00	72.90	. C
MOTA	4594	C	LEU		120	44.856		194.919		77.03	Ċ
ATOM	4595	Ō	LEU			45.129		194.415		76.76	č
ATOM	4596	N	ALA	_		44.078		194.322		76.76	C
ATOM	4597	CA	ALA			43.458				73.80	
								193.025			C
ATOM	4598	CB	ALA			42.311		192.800		73.47	C
ATOM	4599	C	ALA			44.441		191.872		71.28	C
MOTA	4600	0	ALA			44.807		191.269		71.09	С
MOTA	4601	N	LEU				100.016			69.82	C
MOTA	4602	CA	LEU		122	45.788	100.244	190.477	1.00	68.48	C
MOTA	4603	CB	LEU	C	122	46.162	101.725	190.431	1.00	65.97	C
MOTA	4604	CG	LEU	C	122	47.332	102.127	189.535	1.00	67.82	C
MOTA	4605	CD1	LEU	С	122	47.306	101.337	188.240	1.00	68.18	C
ATOM	4606	CD2	LEU	C	122	47.259	103.624	189.274	1.00	69.44	C
ATOM	4607	C	LEU	C	122	47.041	99.390	190.576	1.00	68.66	С
ATOM	4608	0	LEU	C	122	47.872	99.606	191.440	1.00	71.50	C
ATOM	4609	N	PRO	C	123	47.195		189.680		70.18	c
ATOM	4610	CD	PRO			46.281		188.586		72.27	Č.
ATOM	4611	CA	PRO			48.375		189.698		71.13	Č
ATOM	4612	CB	PRO			47.993		188.714		72.33	Č
ATOM	4613	CG	PRO			47.168		187.700		72.84	C
ATOM	4614	C	PRO					189.293			
						49.655				70.11	C
MOTA	4615	0	PRO			49.688		188.277		69.35	C
ATOM	4616	N	PRO			50.728		190.082		68.55	C
MOTA	4617	CD	PRO	_		50.843		191.121		66.12	C
ATOM	4618	CA	PRO			52.027		189.857		68.08	C
ATOM	4619	CB	PRO			53.002		190.638		66.35	C
ATOM	4620	CG	PRO		124	52.235		190.898	1.00	68.45	C
MOTA	4621	C	PRO	C	124	52.449	98.992	188.407	1.00	67.98	С
MOTA	4622	0	PRO	С	124	52.988	100.040	188.059	1.00	66.69	C
MOTA	4623	N	ASP	C	125	52.211	98.004	187.564	1.00	70.69	C
MOTA	4624	CA	ASP	С	125	52.562	98.111	186.152	1.00	76.00	С
ATOM	4625	CB	ASP	C	125	52.093	96.860	185.433	1.00	82.61	С
MOTA	4626	CG	ASP	C	125	50.626	96.577	185.692	1.00	90.11	С
ATOM	4627	OD1	ASP	C	125	49.761	97.326	185.181	1.00	92.24	С
MOTA	4628	OD2	ASP	С	125	50.336		186.429		95.35	C
ATOM	4629	C	ASP			51.869		185.515		76.82	Ċ
ATOM	4630	ō	ASP		125	52.426		184.653		76.53	č
ATOM	4631	Ŋ	GLN			50.644		185.964	1.00		Ċ
ATOM	4632	CA	GLN				100.615			77.88	Č
ATOM	4633	CB	GLN		126		100.086			84.26	č
ATOM	4634	CG	GLN				100.918			90.11	Č
ATOM	4635	CD	GLN		126		100.318			91.50	C
MOTA	4636		GLN				100.222			90.64	Ċ
ATOM			GLN					185.277			C
_	4637					45.895				90.61	_
ATOM	4638	C	GLN				101.953			76.75	C
ATOM	4639	0	GLN				102.698			76.79	C
ATOM	4640	N	ALA				102.275			72.89	C
ATOM	4641	CA	ALA				103.516			67.15	C
ATOM	4642	CB	ALA				103.214			62.36	C
MOTA	4643	C	ALA				104.633			65.58	C
MOTA	4644	0	ALA				105.784			65.29	C
ATOM	4645	N	ALA			53.176	104.307	185.981	1.00	64.51	C
MOTA	4646	CA	ALA	С	128	53.934	105.323	185.259	1.00	66.86	C
MOTA	4647	CB	ALA	С	128	55.050	104.668	184.455	1.00	62.32	С
MOTA	4648	C	ALA	C	128	53.053	106.173	184.338		71.69	C
MOTA	4649	0	ALA				107.393			72.64	C

MOTA	4650	N	GLU	С	129		105.52			1.00 74	.88		C
MOTA	4651	CA	GLU	С	129	51.210	106.21	1 18	2.719	1.00 76	.58		C
MOTA	4652	CB	GLU	С	129	50.205	105.22	3 18	2.140	1.00 82	.30		C
ATOM	4653	CG	GLU	C	129		103.78			1.00 99			C
ATOM	4654	CD	GLU				102.81			1.00105			č
ATOM	4655		GLU				101.59			1.00108			C
ATOM	4656	OE2	GLU				103.27			1.00107			C
MOTA	4657	C	GLU				107.31			1.00 76	.13		C
ATOM	4658	0	GLU	С	129		108.39			1.00 78	.21		C
MOTA	4659	N	LYS	С	130		107.02			1.00 71	.78		С
MOTA	4660	CA	LYS	C	130	49.137	107.97	L 18	5.372	1.00 68	.78		С
ATOM	4661	CB	LYS				107.31			1.00 73			C
ATOM	4662	CG	LYS				105.98			1.00 76			Č
ATOM	4663	CD	LYS	-			106.17			1.00 77			C
ATOM	4664	CE											
			LYS				104.84			1.00 80			C
ATOM	4665	NZ	LYS				105.03			1.00 81			C
ATOM	4666	C	LYS				109.25			1.00 66			C
ATOM	4667	0	LYS .				110.16			1.00 65			C
ATOM	4668	N	LEU	C	131		109.33			1.00 66	.23		C
MOTA	4669	CA	LEU	C	131	51.959	110.50	18	5.602	1.00 67	.46		C
ATOM	4670	CB	LEU	C	131	53.446	110.17	18	5.460	1.00 61	.90		C
ATOM	4671	CG	LEU	С	131	54.348	111.32	18	5.948	1.00 59	.71		С
ATOM	4672		LEU				111.42			1.00 51			Ċ
ATOM	4673		LEU	-			111.094			1.00 52			C
MOTA	4674	C	LEU				111.704			•			
									-	1.00 72			C
ATOM	4675	0	LEU	_			111.72			1.00 77			C
ATOM	4676	N	ARG				112.71			1.00 75			С
ATOM	4677	CA	ARG				113.92			1.00 81			C
ATOM	4678	CB	ARG	С	132	49.296	114.42	184	4.948	1.00 86	.32	٠	C
ATOM	4679	CG	ARG	С	132	48.203	113.37	184	4.812	1.00 94	.44		C
MOTA	4680	CD	ARG	C	132	46.949	113.78	7 18	5.582	1.00101	.07		C
ATOM	4681	NE	ARG	C	132	46.076	112.64	18	5.869	1.00105	.90		C
ATOM	4682	CZ	ARG				112.68			1.00106			Ċ
ATOM	4683		ARG				113.814			1.00104			č
ATOM	4684	NH2					111.59			1.00107			c
ATOM			ARG										c
	4685	C					114.99			1.00 83			
ATOM	4686	0	ARG				114.71			1.00 81			C
ATOM	4687	N	PHE				116.20			1.00 85			C
ATOM	4688	CA	PHE				117.28			1.00 89			С
MOTA	4689	CB	PHE	С	133	53.489	117.35	18:	3.431	1.00 89	.20		C
ATOM	4690	CG	PHE	C	133	54.402	116.16	7 18:	3.348	1.00 90	.91		C
ATOM	4691	CD1	PHE	C	133	53.928	114.93	1 18:	2.914	1.00 91	.02		C
MOTA	4692	CD2	PHE	C	133	55.737	116.27	3 18	3.726	1.00 92	.17		C
ATOM	4693		PHE				113.82			1.00 92			С
ATOM	4694		PHE				115.18			1.00 90			Ċ
ATOM	4695	CZ	PHE				113.94			1.00 91			Č
ATOM	4696		PHE				118.66			1.00 92			C
		C											
ATOM	4697	0	PHE				118.80			1.00 94			C
ATOM	4698	N	ARG				119.67			1.00 94			C
ATOM	4699	CA	ARG				121.07			1.00 97			С
ATOM	4700	CB	ARG				121.35			1.00 94			C
ATOM	4701	CG	ARG	C٠	134	51.710	122.82	18	6.566	1.00 95	.15		C
ATOM	4702	CD	ARG	С	134	51.724	123.03	5 18	8.066	1.00 99	.61		C
ATOM	4703	NE	ARG	C	134	50.655	122.29	18	8.727	1.00102	.22		C
ATOM	4704	CZ	ARG				121.98			1.00102			č
ATOM	4705		ARG				122.35			1.00101			c
ATOM	4705		ARG				121.31			1.00101			C
			ARG				121.83						C
ATOM	4707	С	AKG	C	724	23.644	141.83	TQ.	#.35T	1.00101	. 14		_

	. =	_							_
MOTA	4708	0	ARG C			122.108		1.00101.67	C
ATOM	4709	N	ARG C	135		122.181		1.00103.95	С
ATOM	4710	CA	ARG C	135	55.090	122.853	182.890	1.00105.02	C
MOTA	4711	CB	ARG C	135	55.636	122.184	181.634	1.00105.65	C
ATOM	4712	CG	ARG C	135	54.808	122.423	180.392	1.00104.70	·C
ATOM	4713	CD	ARG C	135		123.246	179.441	1.00106.30	С
ATOM	4714	NE	ARG C			122.623		1.00106.12	č
ATOM	4715	CZ	ARG C			123.255		1.00106.19	č
ATOM			ARG C			122.591			C
	4716							1.00107.56	
ATOM	4717	NH2				124.547		1.00105.16	C
MOTA	4718	C	ARG C			124.353		1.00105.53	C
MOTA	4719	0	ARG C		54.334	124.816	181.750	1.00106.67	C
ATOM	4720	N	SER C	136				1.00105.05	C
ATOM	4721	CA	SER C	136	55.811	126.559	183.360	1.00105.50	С
ATOM	4722	CB	SER C	136	55.920	127.222	184.740	1.00104.11	С
ATOM	4723	OG	SER C	136	54.696	127.143	185.449	1.00103.41	C
MOTA	4724	C	SER C	136	57.050	126.889	182.527	1.00106.70	С
ATOM	4725	0	SER C		57.347	126.200	181.548	1.00107.30	С
ATOM	4726	N	ALA C			127.939		1.00107.29	Č
ATOM	4727	CA	ALA C			128.325		1.00107.41	č
ATOM	4728	CB	ALA C			129.762		1.00106.98	Č
ATOM	4729	CD	ALA C			128.177		1.00107.82	Ċ
ATOM	4730	0	ALA C			128.646		1.00106.77	C
ATOM	4731	N	ASN C			127.513		1.00108.40	C
MOTA	4732	CA	ASN C			127.293		1.00107.89	C
MOTA	4733	CB	ASN C			128.623		1.00108.60	C
MOTA	4734	CG	ASN C	138		129.434		1.00109.12	C
MOTA	4735	OD1	ASN C	138	59.013	128.961	187.070	1.00105.10	С
MOTA	4736	ND2	ASN C	138	59.885	130.667	185.885	1.00106.89	. C
MOTA	4737	C	ASN C	138	60.396	126.284	186.398	1.00105.81	С
ATOM	4738	Ο.	ASN C	138	61.217	125.727	187.125	1.00104.03	C
MOTA	4739	N	SER C	139	59.094	126.033	186.471	1.00104.30	С
ATOM	4740	CA	SER C			125.120		1.00101.96	Č
ATOM	4741	CB	SER C			125.927		1.00101.41	Ċ
ATOM	4742	OG	SER C			127.050		1.00102.22	Č
ATOM	4743	C	SER C			123.960		1.00102.22	č
ATOM	4744	Ö	SER C			123.978		1.00101.72	C
									C
ATOM	4745	N	LEU C			122.951		1.00 97.77	
ATOM	4746	CA	LEU C			121.767		1.00 92.68	C
MOTA	4747	CB	LEU C			120.957		1.00 90.35	C
MOTA	4748	CG	LEU C	140		119.856		1.00 91.97	C
ATOM	4749		LEU C			119.104		1.00 89.68	C
ATOM	4750		LEU C			118.909		1.00 90.76	C
ATOM	4751	С	LEU C		57.314	120.942	187.172	1.00 90.20	C
ATOM	4752	0	LEU C		58.211	120.599	187.938	1.00 92.58	C
ATOM	4753	N	THR C	141	56.049	120.603	187.372	1.00 85.90	C
MOTA	4754	CA	THR C	141	55.664	119.867	188.567	1.00 83.10	С
ATOM	4755	CB	THR C	141	54.619	120.683	189.373	1.00 82.55	C
ATOM	4756		THR C	141		121.966		1.00 82.12	C
ATOM	4757		THR C			119.960		1.00 81.52	C
ATOM	4758	C	THR C			118.450		1.00 82.39	č
ATOM	4759	ō	THR C			118.260		1.00 82.43	Č
ATOM	4760	N	LEU C			117.461		1.00 82.43	G ,
			TEO C			116.057			c
ATOM	4761	CA	TEO C			115.130		1.00 71.84	
ATOM	4762	CB						1.00 66.72	C
MOTA	4763	CG	TEA C			115.145		1.00 69.00	C
MOTA	4764		TEA C	_		114.463		1.00 63.82	C
MOTA	4765	CD2	ren c	142	58.699	116.572	187.944	1.00 67.43	С

•										
MOTA	4766	C	LEU C	142	54.461	115.834	189.259	1.00	72.11	C
MOTA	4767	0	LEU C	142	54.493	116.273	190.408	1.00	70.94	C
MOTA	4768	N -	ILE C	143	53.417	115.167	188.781	1.00	72.83	C
MOTA	4769	CA	ILE C	143	52.244	114.918	189.609	1.00	72.56	C
ATOM	4770	CB	ILE C	143	51.070	115.823	189.170	1.00	73.87	C
MOTA	4771	CG2	ILE C	143	51.135	116.059	187.680	1.00	75.28	С
MOTA	4772	CG1	ILE C	143			189.586	1.00	72.87	C
MOTA	4773	CD1	ILE C	143	49.495	115.186	191.084	1.00	77.03	C
MOTA	4774	С	ILE C	143	51.827	113.457	189.549	1.00	72.54	С
ATOM	4775	0	ILE C	143	51.469	112.947	188.491	1.00	73.64	С
MOTA	4776	N	ASN C	144	51.872	112.795	190.702	1.00	72.15	C
MOTA	4777	CA	ASN C	144	51.524	111.379	190.812	1.00	69.54	С
MOTA	4778	CB	ASN C	144	52.730	110.595	191.346	1.00	67.79	С
ATOM	4779	CG	ASN C	144	52.398	109.159	191.687	1.00	67.15	C
ATOM	4780	OD1	ASN C	144	51.335	108.651	191.333	1.00	66.56	С
ATOM	4781	ND2	ASN C	144	53.320	108.491	192.373	1.00	65.10	С
ATOM	4782	C	ASN C	144	50.312	111.160	191.709	1.00	67.07	C
MOTA	4783	0	ASN C	144	50.370	111.395	192.911	1.00	64.81	C
MOTA	4784	N	PRO C	145	49.192	110.709	191.119	1.00	68.79	C
MOTA	4785	CD	PRO C	145	48.991	110.730	189.656	1.00	68.70	С
ATOM .	4786	CA	PRO. C	145	47.923	110.436	191.804	1.00	68.43	С
MOTA	4787	CB	PRO C	145	46.896	110.812	190.752	1.00	69.14	C
MOTA	4788	CG	PRO C	145	47.554	110.264	189.507	1.00	70.72	С
MOTA	4789	C	PRO C			108.986			68.08	C
MOTA	4790	0	PRO C	145	46.808	108.664	192.986	1.00	69.28	C
MOTA	4791	N	THR C	146	48.645	108.111	191.820	1.00	67.03	C
MOTA	4792	CA	THR C	146	48.575	106.699	192.181	1.00	63.58	C
MOTA	4793	CB	THR C	146	49.526	105.885	191.309	1.00	62.52	C
MOTA	4794	QG1				105.778		1.00	57.38	C
MOTA	4795	CG2	THR C	146	49.728	106.579	189.970	1.00	64.49	C
MOTA	4796	С	THR C	146	48.991	106.527	193.635	1.00	64.63	C
MOTA	4797	0	THR C	146		107.506		1.00	68.21	C
MOTA	4798	N	PRO C			105.280			63.48	C
ATOM	4799	CD	PRO C			104.122			66.45	C
MOTA	4800	CA	PRO C			105.092			60.60	C
ATOM	4801	CB	PRO C			104.133			63.08	C
MOTA	4802	CG	PRO C			103.189			66.43	C
ATOM	4803	С	PRO C			104.505			56.95	С
ATOM	4804	0	PRO C			103.882			55.51	C
ATOM	4805	N	TYR C			104.700			54.74	C
MOTA	4806	CA	TYR C			104.186			54.65	C
ATOM	4807	CB	TYR C			103.179			51.56	C
MOTA	4808	CG	TYR C			102.076			55.39	C
MOTA	4809	CD1	TYR C				192.805		54.49	C
ATOM	4810	CE1					192.740		54.32	C
ATOM	4811		TYR C				193.762		59.71	C
MOTA	4812		TYR C		51.683		193.703		57.62	C
MOTA	4813	CZ	TYR C		50.422		193.195		55.86	C
MOTA	4814	OH	TYR C		49.510		193.180		60.78 52.87	C
ATOM	4815	C	TYR C				194.337			C
MOTA	4816	0	TYR C			106.300			54.93	Ċ
MOTA	4817	N	TYR C				194.897		47.46 42.87	C
MOTA	4818	CA					194.723 195.709			C C
MOTA	4819	CB	TYR C						41.06 43.02	C
MOTA	4820	CG	TYR C				197.044 198.039		46.38	c
ATOM	4821		TYR C				198.039		46.38	C
MOTA	4822		TYR C						47.23	C
MOTA	4823	U)2	TIK	・ スマフ	21.277	107.761	T21.30T	¥ . U U	マノ・ブ生	L

MOTA	4824	CE2	TYR	C	149		57.705	108.425	198.525	1.00	43.85	C
MOTA	4825	CZ	TYR						199.497	1.00	42.45	C
MOTA	4826	OH	TYR	C	149		56.717	108.471	200.700	1.00	44.06	С
MOTA	4827	C	TYR		149		56.862	105.971	193.283	1.00	40.37	С
MOTA	4828	0	TYR		149		57.246	104.892	192.829	1.00	40.63	C
MOTA	4829	N	LEU					107.080		1.00	35.91	C
MOTA	4830	CA	ΓEΩ			•		107.037		1.00	36.47	C
ATOM	4831	CB	LEU		150			107.873	190.284	1.00	37.72	
MOTA	4832	CG	LEU		150			107.390		1.00	44.89	C
ATOM	4833	CD1						108.267			44.46	C
MOTA	4834	CD2	LEU					105.929			45.28	G.
MOTA	4835	C	LEU					107.534			35.58	C
MOTA	4836	0	LEU		150			108.683			34.54	C
MOTA	4837	N	THR					106.654			35.14	C
MOTA	4838	CA	THR					107.029			39.49	C
ATOM	4839	CB	THR					105.850			38.22	C
MOTA	4840	OG1	THR					105.396			35.24	C
ATOM	4841		THR		151			106.295			37.54	· C
MOTA	4842	C	THR					107.453			43.69	C
ATOM	4843	0	THR					106.657			45.08	C
ATOM	4844	И	VAL					108.712			47.76	C
ATOM	4845	CA	VAL					109.279			52.50	C
MOTA	4846	CB	VAL		152			110.604			54.82	C
ATOM ATOM	4847	CG2	VAL					111.283			54.59	C
ATOM	4848 4849	C	VAL VAL					110.346 109.558			52.61 54.39	C
ATOM	4850	0	VAL					110.304			56.59	C
ATOM	4851	N	THR		153			108.954			57.56	c
ATOM	4852	CA	THR					109.140			61.61	C
ATOM	4853	CB	THR					107.882			62.07	c
ATOM	4854	OG1			153			108.091			62.08	C
ATOM	4855	CG2	THR		153	•		106.675			61.10	C
ATOM	4856	C	THR					109.423			66.39	č
ATOM	4857	ō	THR					109.264		1.00		č
ATOM	4858	N	GLU					109.850			69.21	č
MOTA	4859	CA	GLU		154			110.189			71.00	Ċ
ATOM	4860	CB	GLU					108.929			68.39	Ċ
MOTA	4861	CG	GLU		154			108.080			74.25	Ċ
MOTA	4862	CD	GLU	С	154			107.138		1.00	79.00	C
ATOM	4863	OE1	GLU	C	154		68.029	106.383	180.340	1.00	78.01	С
MOTA	4864	OE2	GLU	С	154		66.232	107.160	179.331	1.00	84.26	C
MOTA	4865	С	\mathtt{GLU}	C	154		64.419	111.123	181.650	1.00	72.60	С
MOTA	4866	0	GLU	C	154			110.941		1.00	73.81	C
MOTA	4867	N	LEU	C	155		64.131	112.127	182.472	1.00	74.75	C
MOTA	4868	CA	LEU	C	155		63.098	113.110	182.168	1.00	77.41	C
MOTA	4869	CB	LEU		155			113.835			71.93	С
ATOM	4870	CG	LEU				61.479	114.787	183.332		69.10	C
MOTA	4871	CD1	LEU	С	155			114.000			69.43	C
ATOM	4872	CD2	LEU				61.305	115.530	184.642	1.00	67.56	C
MOTA	4873	С	TEO					114.117			82.70	C
ATOM	4874	0	LEU					114.435		1.00	83.75	C
ATOM	4875	N	ASN					114.620			87.15	C
MOTA	4876	CA	ASN					115.589			89.66	C
MOTA	4877	CB	ASN					114.852			87.16	C
MOTA	4878	CG	ASN					113.775			89.41	C
MOTA	4879		ASN					114.063			91.24	C
MOTA	4880		ASN					112.522			91.32	С
MOTA	4881	С	ASN	С	156		62.181	116.537	178.862	1.00	92.85	С

WO 02/102974 PCT/US01/47994

MOTA	4882	0	ASN	C 156		61.040	116.120	178.643	1.00 90.98	С
ATOM	4883	N	ALA	C 157		62.531	117.816	178.754	1.00 97.40	C
MOTA	4884	CA	ALA	C 157		61.592	118.851	178.334	1.00101.49	C
MOTA	4885	CB	ALA	C 157				178.769	1.00101.71	Č
MOTA	4886	С	ALA	C 157				176.815	1.00104.86	Č
ATOM	4887	0		C 157				176.137	1.00106.02	Ċ
ATOM	4888	N	GLY	C 158				176.296	1.00107.96	Č
ATOM	4889	CA		C 158				174.867	1.00109.79	C
ATOM	4890	С		C 158				174.338	1.00111.23	C
ATOM	4891	ō		C 158				173.783	1.00110.98	C
ATOM	4892	N		C 159			117.983		1.00113.28	c
ATOM	4893	CA		C 159				174.071	1.00115.67	C
ATOM	4894	СВ		C 159				173.072	1.00116.95	c
ATOM	4895	OG1		C 159				173.725	1.00119.65	c
ATOM	4896	CG2		C 159				171.870	1.00118.58	c
ATOM	4897	C		C 159				175.275	1.00116.35	C
ATOM	4898	ō		C 159				175.457	1.00116.33	c
ATOM	4899	N	ARG					176.090	1.00116.21	C
ATOM	4900	CA		C 160				177.289	1.00110.32	C
ATOM	4901	CB		C 160				177.940	1.00122.92	Ċ
MOTA	4902	CG		C 160				179.117	1.00122.32	C
ATOM	4903	CD		C 160				178.652	1.00131.21	C
ATOM	4904	NE	ARG					179.738	1.00130.40	C
ATOM	4905	CZ		C 160				180.628	1.00140.29	C
ATOM	4906	NH1					120.554		1.00140.43	C
ATOM	4907		ARG				122.587		1.00139.43	c
ATOM	4908	C		C 160			118.120		1.00139.43	c
ATOM	4909	ō		C 160			117.590		1.00114.88	C
ATOM	4910	N		2 161			117.727		1.00114.15	. C
ATOM	4911	CA		2 161			116.646		1.00107.63	C
ATOM	4912	CB		161			115.759		1.00107.03	C
ATOM	4913		VAL (116.601		1.00110.07	C
ATOM	4914		VAL (114.617		1.00109.02	C
ATOM	4915	C		2 161			117.248		1.00103.02	c
ATOM	4916	ŏ		2 161			118.160		1.00103.14	C
ATOM	4917	N		C 162			116.740		1.00103.82	C
ATOM	4918	CA		C 162			117.260		1.00 97.88	C
MOTA	4919	CB		C 162			117.495		1.00 93.66	C
ATOM	4920	CG		162			118.520		1.00 91.72	c
ATOM	4921		LEU				118.716		1.00 88.89	c
ATOM	4922		LEU				119.830		1.00 90.96	c
MOTA	4923	C		162			116.390		1.00 90.67	č
ATOM	4924	ō		C 162			115.504		1.00 90.29	c
ATOM	4925	N		C 163			116.660	185.765	1.00 86.34	c
ATOM	4926	CA		C 163	_		115.925		1.00 82.23	C
ATOM	4927	CB	GLU (•		116.915		1.00 86.91	C
ATOM	4928	CG		C 163			116.325		1.00 94.31	_
ATOM	4929	CD		C 163			117.359		1.00 97.20	C C
ATOM	4930		GLU (117.709		1.00 95.31	c
ATOM	4931		GLU (69 049	117.828	190 853	1.00 99.85	c
ATOM	4932	C		C 163			114.966		1.00 75.97	C
ATOM	4933	Ö		C 163			115.325		1.00 75.64	c
ATOM	4934	N		C 164			113.741		1.00 /5.84	C
ATOM	4935	CA		C 164			112.698		1.00 67.24	C
MOTA	4936	CB		C 164			111.501		1.00 59.92	
MOTA	4936	CG		C 164			111.501		1.00 59.24	C
ATOM	4937		ASN (110.591		1.00 62.11	C
ATOM	4939		ASN (111.326		1.00 63.06	C
WIO!!	モノンン	14772	"STATA "	- TOZ		00.702	~~~~~	100.020	1.00 00.73	С

					•						
MOTA	4940	C	ASN	_			113.161		1.00	56.66	C
ATOM	4941	0	ASN	С	164	64.967	114.114	190.043	1.00	59.30	C
MOTA	4942	N	ALA	С	165	63.548	112.482	189.493	1.00	51.93	С
ATOM	4943	CA	ALA	C	165	62.635	112.864	190.546	1.00	49.65	С
ATOM	4944	CB	ALA	С	165	61.572	113.788	190.003	1.00	52.53	C
MOTA	4945	С	ALA	С	165	61.997	111.641	191.167	1.00	50.47	C
ATOM	4946	0	ALA	С	165	61.908	110.580	190.544	1.00	50.53	C
ATOM	4947	N	LEU	С	166		111.801		1.00	46.38	C
MOTA	4948	CA	LEU	С	166	60.923	110.746	193.159	1.00	43.58	C
MOTA	4949	CB	LEU	С	166			194.408	1.00	36.70	C
ATOM	4950	CG	LEU	С	166			195.357		44.53	Ċ
ATOM	4951	CD1	LEU		166		108.027			36.17	Ċ
ATOM	4952		LEU		166		109.216			33.99	Ċ
ATOM	4953	C	LEU				111.337			44.39	Č
ATOM	4954	ō	LEU		166		112.201			44.64	č
ATOM.	4955	N	VAL		167		110.888			45.73	Č
ATOM	4956	CA	VAL		167		111.455			45.36	č
ATOM	4957	CB	VAL				111.732			44.90	Č
ATOM	4958	CG1					112.544			47.30	Ċ
ATOM	4959	CG2			167		112.470			40.79	Ċ
ATOM	4960	C	VAL		167		110.596			45.36	C
MOTA	4961	Ö	VAL				109.508			48.17	C
ATOM	4962	N	PRO				111.098			46.56	C
ATOM	4963	CD	PRO		168			195.704		44.33	, c
ATOM	4964	CA	PRO		168		110.448			49.57	. c
ATOM	4965	CB	PRO		168		111.454			49.44	G
ATOM	4966	CG	PRO				112.774			49.37	c
ATOM	4967	C	PRO				110.122			53.61	. 0
ATOM	4968	o	PRO	_	168		110.122			54.91	
ATOM		и .	PRO		169		100.002				C
ATOM	4969 4970	CD	PRO		169		108.184			56.47 60.09	c
MOTA	4971	CA	PRO				108.602			58.83	C
ATOM	4972	CB	PRO				107.495			59.06	
ATOM	4973	CG	PRO		169		107.433			62.55	
ATOM	4974	C	PRO				109.720			60.12	C
ATOM	4975	0	PRO				110.473			61.83	c
ATOM	4976	N	MET				109.822			60.48	C
ATOM	4977	CA	MET				110.853			57.07	
ATOM	4978	CB	MET		170		110.653			57.40	C
ATOM	4979	CG	MET				109.243		1.00		c
ATOM	4980	SD	MET		170		109.243		1.00		C
ATOM	4981	CE	MET		170		106.857			81.52	C
ATOM	4982	C	MET				112.177		•	55.70	C
ATOM	4983	0	MET		170		112.939			54.26	C
ATOM	4984	N	GLY				112.437			53.79	c
ATOM	4985	CA	GLY				113.661	_		57.23	C
ATOM	4986	CA	GLY				114.207			62.42	_
ATOM			GLY								C
ATOM	4987	O N	GLU				113.817 115.101			65.08 65.84	C
ATOM	4988	N	GLU								C
MOTA	4989 4990	CA CB	GLU				115.695 116.742			69.49 74.68	C
ATOM										80.71	
	4991	CG	GLU				117.710				C
ATOM	4992	CD	GLU				118.526			86.58	C
ATOM	4993		GLU				119.305			87.16	C
MOTA	4994		GLU				118.383 116.317			90.77	C
MOTA	4995	C	GLU							68.52	C
MOTA	4996	0	GLU				116.574			67.20	C
MOTA	4997	N	SER	C	173	55.889	116.555	192.937	T.00	70.89	. С

										•	
MOTA	4998	CA	SER	C	173	`	57.215	117.134	193.090	1.00 74.44	C
MOTA	4999	CB	SER	C	173		58.267	116.024	193.079	1.00 73.77	C
ATOM	5000	OG	SER	C	173		57.754	114.843	193.673	1.00 81.48	C
ATOM	5001	C	SER	C,	173		57.469	118.076	191.920	1.00 76.32	C
ATOM	5002	0	SER	С	173		57.007	117.824	190.806	1.00 74.84	C
ATOM	5003	N	ALA	C	174				192.167	1.00 79.34	Ċ
ATOM	5004	CA			174				191.104	1.00 81.62	č
ATOM	5005	CB			174				191.502	1.00 78.56	Č
ATOM	5006	C	ALA						190.769	1.00 82.90	C
ATOM	5007	ō	ALA								
ATOM	5008	N	VAL						191.614	1.00 84.86	C
ATOM		CA							189.544	1.00 84.83	C
	5009				175				189.091	1.00 90.74	C
ATOM	5010	CB	VAL						188.104	1.00 91.39	C
ATOM	5011		VAL						187.437	1.00 85.34	С
ATOM	5012		VAL						188.814	1.00 91.28	C
ATOM	5013	C	VAL		175				188.374	1.00 95.84	C
MOTA	5014	0	VAL						187.573	1.00 97.42	С
MOTA	5015	N	LYS						188.677	1.00 98.31	C
MOTA	5016	CA	LYS				63.317	123.077	188.060	1.00101.27	·C
MOTA	5017	CB	LYS	С	176		64.706	123.587	188.455	1.00100.69	С
MOTA	5018	CG	LYS	C	176		64.846	123.986	189.934	1.00103.93	С
MOTA	5019	CD	LYS				64.767	122.775	190.880	1.00100.95	С
MOTA	5020	CE	LYS	C	176		65.184	123.136	192.311	1.00 93.35	С
MOTA	5021	NZ	LYS	С	176		64.327	124.214	192.885	1.00 85.34	C
MOTA	5022	C	LYS	C	176		63.239	122.973	186.534	1.00105.72	C
ATOM	5023	0	LYS	С	176		64.022	122.258	185.906	1.00105.99	C
MOTA	5024	N	LEU	C	177		62.280	123.688	185.947	1.00109.01	Ċ
MOTA	5025	CA	LEU	C	177				184.498	1.00111.62	Ċ
ATOM	5026	CB	LEU	-	177				184.244	1.00108.02	Ċ
ATOM	5027	CG	LEU						182.824	1.00106.91	č
ATOM	5028		LEU						182.042	1.00106.49	Č
	5029		LEU						182.898	1.00106.11	Č
ATOM	5030	C	LEU						183.883	1.00114.77	č
ATOM	5031	ō	LEU						184.072	1.00114.63	Č.
ATOM	5032	N	PRO						183.123	1.00118.03	Ċ
ATOM	5033	CD	PRO						182.734	1.00118.62	c
ATOM	5034	CA	PRO					125.080		1.00110.02	ď
ATOM	5035	CB	PRO			•			181.858	1.00121.31	G
ATOM	5036	CG	PRO						181.481	1.00113.30	C
ATOM	5037	C	PRO						181.399	1.00121.21	C
ATOM	5038	ō	PRO						181.096	1.00125.09	C
ATOM	5039	N	SER						180.837		
ATOM	5040	CA	SER	_						1.00127.68	C
	5041								179.799	1.00129.15	C
ATOM		CB	SER						180.184	1.00130.38	C
ATOM	5042	OG	SER					129.226		1.00132.50	C
ATOM	5043	C	SER	-		•		126.590		1.00129.00	C
ATOM	5044	0	SER						177.389	1.00128.49	C
ATOM	5045	И	ASP						178.331	1.00128.89	C
MOTA	5046	CA	ASP						177.054	1.00127.75	C
ATOM	5047	CB	ASP					124.741		1.00128.01	C
ATOM	5048	CG	ASP					125.752		1.00127.52	C
ATOM	5049		ASP					125.363		1.00126.48	C
MOTA	5050		ASP						177.939	1.00125.39	С
MOTA	5051	C	ASP						176.687	1.00126.58	C
MOTA	5052	0	ASP						176.041	1.00125.43	С
· MOTA	5053	N	ALA					124.471		1.00125.71	C
MOTA	5054	CA	ALA				61.768	123.655	177.100	1.00124.62	C
ATOM	5055	CB	ALA	C	181		60.615	124.492	177.544	1.00123.97	C

ATOM	5056	С	ALA C	181	61.388	122.968	175.801	1.00124.67	С
ATOM	5057	0	ALA C	181	62.219	122.587	174.974	1.00123.68	. C
ATOM	5058	N	GLY C	182	60.075	122.763	175.719	1.00125.40	C
ATOM	5059	CA	GLY C	182	59.389	122.130	174.611	1.00126.58	С
ATOM	5060	C	GLY C	182	57.968	121.923	175.103	1.00127.55	С
MOTA	5061	0	GLY C	182	57.167	122.860	175.133	1.00129.15	С
MOTA	5062	N	SER C	183	57.685	120.696	175.517	1.00126.04	C
ATOM	5063	CA	SER C	183	56.393	120.289	176.035	1.00123.78	C
ATOM	5064	СВ	SER C	183		121.005		1.00124.79	C
MOTA	5065	OG	SER C	183		121.012		1.00126.40	Ċ
ATOM	5066	C	SER C	183	56.384	118.825	175.675	1.00121.59	C
MOTA	5067	Ō	SER C	183		118.058		1.00120.48	č
ATOM	5068	N	ASN C	184		118.457		1.00119.90	Ċ
ATOM	5069	CA	ASN C			117.084		1.00118.04	Ċ
ATOM	5070	CB	ASN C	184	58.587	117.034	173.281	1.00117.77	Ċ
ATOM	5071	CG	ASN C			115.612		1.00117.70	Ċ
ATOM	5072		ASN C	184		114.873		1.00118.37	Ċ
ATOM	5073		ASN C			115.222		1.00117.12	Ċ
ATOM	5074	С	ASN C			116.366		1.00115.09	. C
ATOM	5075	0	ASN C			115.599		1.00114.37	C
ATOM	5076	N	ILE C	185		116.652		1.00111.78	C
ATOM	5077	CA	ILE C		58.061	116.041	178.057	1.00107.86	Ċ
ATOM	5078	CB	ILE C			116.358		1.00106.83	C
ATOM	5079		ILE C			115.695		1.00107.60	Ċ
ATOM	5080		ILE C			117.874		1.00103.38	Ċ
ATOM	5081		ILE C			118.292		1.00100.79	Ċ
ATOM	5082	С	ILE C			114.526		1.00104.91	C
ATOM	5083	0	ILE C			113.861		1.00104.46	C
ATOM	5084	N	THR C		59.347	113.994	178.192	1.00 99.88	, G
ATOM	5085	CA	THR C	186		112.572		1.00 93.45	Č
ATOM	5086		THR C			112.356		1.00 90.46	C
ATOM	5087	OG1	THR C	186	61.627	113.268	176.956	1.00 91.77	, C
MOTA	5088		THR C		59.794	112.624	175.582	1.00 91.80	Ċ
ATOM	5089	C	THR C		60.237	111.972	179.298	1.00 89.73	С
ATOM	5090	0	THR C		61.086	112.598	179.941	1.00 88.73	C
MOTA	5091	N	TYR C		59.831	110.751	179.636	1.00 84.51	С
MOTA	5092	CA	TYR C	187	60.343	110.119	180.843	1.00 76.69	С
ATOM	5093	CB	TYR C	187	59.608	110.688	182.040	1.00 70.63	C
ATOM	5094	CG	TYR C	187	58.169	110.248	182.070	1.00 65.83	С
MOTA	5095	CD1	TYR C	187	57.813	108.990	182.552	1.00 67.66	C
ATOM	5096	CE1	TYR C	187	56.496	108.564	182.554	1.00 64.58	C
MOTA	5097	CD2	TYR C		57.166	111.071	181.588	1.00 66.42	С
MOTA	5098	CE2	TYR C	187	55.842	110.656	181.584	1.00 66.81	С
ATOM	5099	CZ	TYR C	187	55.515	109.402	182.069	1.00 66.60	C
MOTA	5100	OH	TYR C	187	54.202	108.998	182.072	1.00 69.08	С
MOTA	5101	C	TYR C	187	60.169	108.616	180.876	1.00 74.04	C
MOTA	5102	0	TYR C	187	59.268	108.067	180.249	1.00 75.77	C
ATOM	5103	N	ARG C		61.030	107.962	181.644	1.00 71.58	С
MOTA	5104	CA	ARG C		60.966	106.519	181.852	1.00 66.93	C
MOTA	5105	CB	ARG C	188	62.210	105.844	181.279	1.00 66.96	С
MOTA	5106	CG	ARG C			106.217		1.00 73.84	C
ATOM	5107	CD	ARG C			105.699		1.00 76.28	Ċ
MOTA	5108	NE	ARG C			104.246		1.00 83.41	C
MOTA	5109	CZ	ARG C		63.207	103.555	178.347	1.00 86.78	C
MOTA	5110		ARG C			104.189		1.00 86.61	C
MOTA	5111		ARG C			102.230		1.00 89.02	C
MOTA	5112	C	ARG C			106.425		1.00 63.56	Č
MOTA	5113	0	ARG C			107.431		1.00 66.39	Ċ

ATOM	5114	N	THR (189	60.666	105.265	183.948	1.00 56.26	. с
ATOM	5115	CA	THR (189	60.709	105.175	185.406	1.00 51.73	С
ATOM	5116	CB	THR (189	59.328	105.165	186.053	1.00 44.57	C
ATOM	5117	OG1	THR (189	58.750	103.867	185.906	1.00 40.53	C
MOTA	5118	CG2	THR C	189	58.444	106.219	185.435	1.00 44.58	С
ATOM	5119	C	THR (189	61.431	103.921	185.850	1.00 52.18	C
ATOM	. 5120	0	THR (189	61.963	103.178	185.023	1.00 54.16	C
ATOM	5121	N	ILE (190	61.461	103.687	187.159	1.00 48.53	C
ATOM	5122	CA	ILE (190	62.142	102.517	187.674	1.00 42.95	C
ATOM	5123	CB	ILE (63.328	102.952	188.545	1.00 37.82	C
ATOM	5124	CG2	ILE (190	64.168	101.754	188.935	1.00 36.28	C
ATOM	5125	CG1	ILE (190		103.942		1.00 37.12	С
ATOM	5126	CD1	ILE (190	65.488	104.346	188.358	1.00 25.84	С
ATOM	5127	C	ILE (61.155	101.635	188.424	1.00 44.75	C
ATOM	5128	0	ILE (60.578	102.032	189.439	1.00 48.31	С
MOTA	5129	N	ASN (191	60.947	100.433	187.897	1.00 42.33	С
ATOM ·	5130	CA	ASN C	191	60.003	99.496	188.490	1.00 40.95	С
MOTA	5131	CB	ASN (191	59.467	98.550	187.426	1.00 42.10	C
MOTA	5132	CG	ASN C	191	60.565	97.712	186.800	1.00 44.85	C
MOTA	5133	OD1	ASN (191	61'.391	97.099	187.491	1.00 46.32	С
MOTA	5134	ND2	ASN C	191	60.578		185.485	1.00 45.05	C
ATOM	5135	С	ASN (191	60.592	98.653	189.605	1.00 37.68	С
MOTA	5136	0	ASN C	: 191	61.810	98.641	189.834	1.00 36.56	С
MOTA	5137	N	ASP (59.687	97.925	190.252	1.00 29.54	С
MOTA	5138	CA	ASP (192	59.980		191.355	1.00 26.12	. С
ATOM	5139	CB	ASP (192	58.794	96.105	191.590	1.00 29.81	C
MOTA	5140	CG	ASP (192	57.530	96.835	192.038	1.00 37.12	C
MOTA	5141	OD1	ASP (192	56.574	96.135	192.421	1.00 38.10	C
MOTA	5142	OD2	ASP (192	57.482	98.084	192.017	1.00 41.01	С
ATOM	5143	C	ASP (192	61.221	96.184	191.158	1.00 30.47	С
ATOM	5144	0	ASP (61.752	95.623	192.115	1.00 31.14	С
MOTA	5145	N	TYR C	193	61.698	96.069	189.926	1.00 34.05	С
MOTA	5146	CA	TYR (193	62.862	95.228	189.682	1.00 37.89	C
ATOM	5147	CB	TYR C	193	62.568	94.254	188.547	1.00 39.92	С
MOTA	5148	CG	TYR C	193	61.238	93.590	188.748	1.00 42.75	C
MOTA	5149	CD1	TYR (193	60.125	93.989	188.016	1.00 43.39	C
MOTA	5150	CE1	TYR C	193	58.869	93.439	188.264	1.00 49.48	С
MOTA	5151	CD2	TYR C	193	61.069	92.619	189.738	1.00 45.79	C
MOTA	5152	CE2	TYR (193	59.820	92.062	189.997	1.00 48.41	C
MOTA	5153	CZ	TYR (193	58.723	92.475	189.255	1.00 48.31	С
MOTA	5154	OH	TYR (193	57.484	91.926	189.495	1.00 48.52	С
MOTA	5155	С	TYR (193	64.059	96.066	189.369	1.00 39.57	С
ATOM	5156	0	TYR (193	65.084	95.565	188.902	1.00 39.00	C
MOTA	5157	N	GLY (194	63.919	97.354	189.649	1.00 42.47	С
MOTA	5158	CA	GLY (194	65.006	98.275	189.411	1.00 46.94	С
MOTA	5159	С	GLY (65.286	98.314	187.938	1.00 46.53	C
MOTA	5160	0	GLY (194	66.421	98.531	187.511	1.00 42.21	С
MOTA	5161	N	ALA (195	64.224	98.093	187.170	1.00 50.72	C
MOTA	5162	CA	ALA (64.296		185.720	1.00 53.38	C
MOTA	5163	CB	ALA (195	63.659		185.193	1.00 56.76	C
MOTA	5164	C	ALA (63.592		185.140	1.00 53.03	C
MOTA	5165	0	ALA (62.570	99.761	185.670	1.00 45.75	C
MOTA	5166	N	LEU (196	64.162	99.860	184.065	1.00 57.23	C
MOTA	5167	CA	LEU (196		101.036		1.00 61.31	C
MOTA	5168	CB	LEU (196	64.627	101.616	182.406	1.00 61.57	C
MOTA	5169	CG.	LEU (102.392		1.00 66.94	C
MOTA	5170	CD1	LEU (196		102.733		1.00 63.88	C
MOTA	5171	CD2	LEU (196	65.333	103.655	183.638	1.00 63.34	C

MOTA	5172	C	LEU C		62.354	100.679		1.00 64.83	C
MOTA	5173	0	LEU C		62.350	99.756	181.827	1.00 70.03	С
ATOM	5174	N	THR C	197	61.275	101.400	182.894	1.00 66.18	C
ATOM	5175	CA	THR C	197	60.047	101.125	182.181	1.00 66.57	С
MOTA	5176	CB	THR C	197	58.826	101.751	182.880	1.00 65.48	C
MOTA	5177	OG1	THR C	197	58.916	103.182	182.833	1.00 63.03	C
ATOM	5178	CG2	THR C	197	58.760	101.278	184.324	1.00 63.15	C
ATOM	5179	C	THR C	197	60.242	101.747	180.807	1.00 69.53	C
ATOM	5180	0	THR C	197		102.457		1.00 67.83	c
ATOM	5181	N	PRO C			101.477		1.00 72.51	. č
ATOM	5182	CD	PRO C			100.578		1.00 71.55	Č
ATOM	5183	CA	PRO C			102:058		1.00 74.44	c
ATOM	5184	CB	PRO C			101.235		1.00 73.13	C
ATOM	5185	CG	PRO C			100.955		1.00 71.33	c
ATOM	5186	C	PRO C			103.554		1.00 75.99	C
ATOM	5187	Õ	PRO C			103.334		1.00 75.66	C
ATOM	5188	N	LYS C			104.026		1.00 76.63	c
ATOM .	5189	CA	LYS C	-		104.284		1.00 75.31	C
ATOM	5190	CB	LYS C			105.730			
ATOM	5191		LYS C					1.00 73.36	C
ATOM		CD	LYS C			107.635		1.00 78.70	C
ATOM	5192			-	· · - -	107.963		1.00 84.97	C
	5193	CE	LYS C			109.156		1.00 87.72	C
ATOM	5194	NZ	LYS C			110.446		1.00 84.39	C
ATOM	5195	C	LYS C			106.110		1.00 74.66	C
ATOM ATOM	5196	0	LYS C	_		105.522		1.00 76.81	C
	5197	N	MET C			107.081		1.00 75.62	C
ATOM	5198	CA	MET C			107.512		1.00 76.90	C
ATOM	5199	CB	MET C			107.175		1.00 79.40	· C
ATOM	5200	CG	MET C			106.183		1.00 84.53	C
ATOM	5201	SD	MET C			105.376		1.00 94.91	C
ATOM	5202	CE	MET C			103.653		1.00 91.76	C
ATOM	5203	C .	MET C			109.011		1.00 76.45	C
ATOM	5204		MET C			109.679		1.00 75.14	C
ATOM	5205	N	THR C			109.536		1.00 76.88	C
ATOM	5206	CA	THR C			110.966		1.00 77.61	. C
ATOM	5207	CB	THR C			111.218		1.00 76.28	C
ATOM	5208		THR C			110.584		1.00 74.52	C
ATOM	5209	CG2	THR C			112.715		1.00 73.93	C
ATOM	5210	C	THR C			111.782		1.00 76.90	C
ATOM	5211	0	THR C			111.410		1.00 76.37	C
ATOM	5212	N	GLY C			112.904		1.00 77.52	C
ATOM	5213	CA	GLY C			113.784		1.00 81.83	C
ATOM ATOM	5214 5215	C	GLY C			114.189		1.00 85.10	C
ATOM	-	0	GLY C			114.537		1.00 85.51	C
ATOM	5216 5217	N	VAL C			114.147		1.00 87.70	C
		CA				114.490		1.00 89.74	C
ATOM	5218	CB	VAL C			113.223		1.00 88.84	C
ATOM	5219		VAL C			113.548		1.00 85.33	C
ATOM ATOM	5220		VAL C			112.161		1.00 85.34	C
	5221	C				115.497		1.00 93.55	C
ATOM	5222	0	VAL C			115.138		1.00 96.77	C
ATOM	5223	N	MET C			116.755		1.00 95.77	C
ATOM	5224	CA	MET C			117.826		1.00 98.27	C
MOTA	5225	CB	MET. C			119.198		1.00100.85	C
ATOM	5226	CG	MET C			119.467		1.00106.92	C
ATOM	5227	SD	MET C			118.333		1.00114.76	C
ATOM	5228	CE	MET C	204	52.536	119.164		1.00110.79	C
MOTA	5229	C	MET C	204	48.920	117.763	T8T-628	1.00 97.63	C

MOTA	5230	0	MET	С	204		48.040	117.606	180.822	1.00 96.53	C
ATOM	5231	N	GLU	C	205		48.662	117.880	182.956	1.00 99.36	C
ATOM	5232	CA	GĽU	C	205		47.295	117.841	183.458	1.00102.30	C
ATOM	5233	CB	GLU	C	205		47.241	117.308	184.894	1.00106.56	C
MOTA	5234	CG	GLU	С	205		47.761	118.284	185.952	1.00114.04	C
ATOM	5235	CD	GLU	C	205			118.527		1.00117.38	C
MOTA	5236	OE1	GLU	С	205		47.091	119.296	188.021	1.00117.73	C
MOTA	5237	OE2	GLU	C	205		45.656	117.949	187.037	1.00117.98	C
MOTA	5238	C	GLU	С	205		46.735	119.251	183.430	1.00102.90	C
MOTA	5239	0	GLU	C	205			119.399		1.00102.02	C
MOTA	5240	OXT	GLU	С	205		47.488	120.185	183.792	1.00104.63	С
MOTA	5241	CB	PHE	D	1		57.259	55.852	168.279	1.00 36.89	D
ATOM	5242	CG	PHE	D	1		57.904	56.830	169.212	1.00 36.42	. D
ATOM	5243	CD1	PHE	D	1		58.083	58.162	168.840	1.00 38.81	D
MOTA	5244	CD2	PHE	D	1		58.291	56.437	170.485	1.00 39.03	D
ATOM	5245	CE1	PHE	D	1		58.630	59.083	169.723	1.00 30.53	D
ATOM	5246	CE2	PHE	D	1		58.844	57.353	171.383	1.00 31.99	D
ATOM	5247	CZ	PHE	D	1		59.011	58.680°	170.996	1.00 35.83	D
ATOM	5248	C	PHE	D	1		55.160	57.227	168.009	1.00 32.04	D
ATOM	5249	0	PHE	D	1		55.302	57.704	166.893	1.00 29.74	D
ATOM	5250	N	PHE		1		55.170	54.904	167.334	1.00 41.01	D
MOTA	5251	CA	PHE		1		55.720	55.855	168.338	1.00 36.16	D
MOTA	5252	N	ALA		2		54.499	57.841	168.983	1.00 32.31	D
ATOM	5253	CA	ALA		2		53.909		168.807	1.00 29.54	D
ATOM	5254	CB	ALA		2		52.482		168.380	1.00 22.02	D
ATOM	5255	С	ALA		2		53.988		170.119	1.00 29.62	D
ATOM	5256	Ο.	ALA		2		54.118		171.191	1.00 30.32	D
MOTA	5257	N	CYS		3		53.903		170.044	1.00 25.22	D
ATOM	5258	CA	CYS		. 3		53.978		171.250	1.00 25.37	D
ATOM	5259	C	CYS		3		52.871		171.263	1.00 26.10	D
ATOM	5260	0	CYS		3		52.303		170.233	1.00 28.50	D
ATOM	5261	CB	CYS		3		55.330		171.333	1.00 29.28	D
ATOM	5262	SG	CYS		3		56.828		171.199	1.00 39.44	D
ATOM	5263	N	LYS		4		52.553		172.437	1.00 29.28	D
ATOM	5264	CA	LYS		4		51.523		172.548	1.00 33.89	D
ATOM	5265	CB	LYS		4		50.165		172.936	1.00 32.29	D
ATOM	5266	CG	LYS		4		50.124		174.338	1.00 45.50	D
ATOM	5267	CD	LYS		4		48.805		174.661	1.00 51.16	D
ATOM	5268	CE	LYS		4		47.638		174.816	1.00 56.15	D
ATOM	5269	NZ	LYS		4		47.300		173.535	1.00 65.92	. D
ATOM ATOM	5270 5271	C 0	LYS		4		51.930		173.586 174.448	1.00 37.28 1.00 35.47	D
ATOM	5271		THR		5		52.777		173.487		D
ATOM	5272	N CA	THR		5		51.284 51.549		174.357	1.00 40.33 1.00 37.06	D D
ATOM	5274	CB	THR		5		51.693		173.492	1.00 37.00	D D
ATOM	5275	OG1	THR	-	5		52.879		173.492	1.00 33.03	D
ATOM	5276	CG2			5		50.502		173.596	1.00 37.40	D
ATOM	5277	C	THR		5		50.430		175.377	1.00 36.30	D
ATOM	5278	ō	THR		5		49.260		175.053	1.00 38.39	D
ATOM	5279	N	ALA		6		50.809		176.624	1.00 35.55	D
ATOM	5280	CA	ALA		6		49.860		177.719	1.00 33.33	D
ATOM	5281	CB	ALA		6		50.579		178.996	1.00 35.68	D
ATOM	5282	C	ALA		6	••	48.779		177.410	1.00 38.31	D
ATOM	5283	Ö	ALA		. 6		47.663		177.911	1.00 38.31	ם
ATOM	5284	N	ASN		7		49.115		176.571	1.00 44.27	D
ATOM	5285	CA	ASN		7		48.174		176.371	1.00 48.59	D D
ATOM	5286	CB	ASN		7	-	48.912		175.502	1.00 51.23	D
ATOM	5287	CG	ASN		7		48.371		175.881	1.00 57.00	D
					•				_,_,_,		20

MOTA	5288		ASN		7		47.359	73.923	176.586	1.00	61.41	D
MOTA	5289	ND2	ASN	D	7		49.034		175.419	1.00	45.59	D
ATOM	5290	C	ASN		7		47.120		175.260	1.00	49.26	D
MOTA	5291	0	asn		7		45.948		175.327	1.00	54.86	D
MOTA	5292	N	GLY		8		47.558		174.388		47.30	D
MOTA	5293	CA	GLY	D	8		46.659		173.446	1.00	52.30	D
MOTA	5294	C	GLY	D	8		47.332	68.681	172.216	1.00	57.17	D
MOTA	5295	0	GLY	D	8		47.081		171.881	1.00	59.28	D
MOTA	5296	N	THR		9		48.191		171.555	1.00	52.59	D
ATOM	5297	CA	THR	D	9		48.865		170.318	1.00	47.80	D
ATOM	5298	CB	THR		9		49.710		169.811	1.00	49.09	D
MOTA	5299	OG1			9		48.871		169.659		59.62	D
ATOM	5300	CG2	THR		9		50.327		168.468		51.33	D
MOTA	5301	C	THR		9		49.694		170.266		46.47	D
ATOM	5302	0	THR		9		50.365		171.223		47.30	D
ATOM	5303	N	ALA		10		49.644		169.110		43.63	D
ATOM	5304	CA	ALA		10		50.347		168.881		38.68	D
ATOM	5305	CB	ALA		10		49.343		168.749		28.38	D
ATOM	5306	C	ALA		10		51.215		167.650		38.13	D
ATOM	5307	0	ALA		10		51.013		166.731		42.10	D
ATOM	5308	N	ILE		11		52.193		167.647		35.07	D
ATOM	5309	CA	ILE		11		53.061		166.501		33.71	D
ATOM	5310	CB	ILE		11		54.501		166.810		33.38	D
ATOM	5311	CG2	ILE		11		55.324 54.633		165.545		34.59	D
ATOM	5312	CG1	ILE		11				167.333		34.65	D
ATOM	5313	CD1			11		56.046		167.709 166.268		36.71 34.43	D
ATOM	5314 5315	С 0	ILE		11 11		52.898 53.236	-	167.123		40.94	D D
ATOM	5316	N	PRO		12		52.372		165.108		31.48	D
ATOM ATOM	5317	CD	PRO		12		51.959		163.108		35.92	D
ATOM	5318	CA	PRO		12		52.147		164.782		31.33	D
ATOM	5319	CB	PRO		12		51.135		163.651		35.15	. D
ATOM	5320	CG	PRO		12		51.669		162.868		36.13	D
ATOM	5321	C	PRO		12		53.348		164.385		31.60	Ď
ATOM	5322	ō	PRO		12		54.466		164.304		29.52	D
ATOM	5323	N	ILE		13	`	53.069		164.141		31.67	Ď
ATOM	5324	CA	ILE		13		54.040		163.700		31.87	D
ATOM	5325	CB	ILE		13		53.314		163.279		32.42	D
ATOM	5326	CG2	ILE		13		54.258		162.495		34.06	D
ATOM	5327	CG1	ILE		13		52.741		164.517		27.64	D
ATOM	5328	CD1	ILE	D	13		51.986	55.157	164.210	1.00	23.75	D
ATOM	5329	С	ILE	D	13		54.753	58.953	162.483	1.00	33.11	D
MOTA	5330	0	ILE	D	13		54.092	59.437	161.571	1.00	36.32	D
ATOM	5331	N	GLY	D	14		56.084	58.899	162.466	1.00	30.35	. D
MOTA	5332	CA	GLY	D	14		56.827	59.432	161.337	1.00	30.86	D
MOTA	5333	C	GLY	_	14		57.452		161.631		35.11	D
MOTA	5334	0	GLY		14		58.229		160.832		37.52	D
MOTA	5335	N	GLY		15		57.096		162.775	1.00	34.23	D
MOTA	5336	CA	GLY		15		57.662	62.642	163.161		31.45	D
MOTA	5337	C	GLY		15		56.914		162.695		32.59	D
ATOM	5338	0	GLY		15		55.895		162.014		36.23	מ
ATOM	5339	N	GLY		16	•	57.443		163.064		30.04	D
MOTA	5340	CA	GLY		16		56.828		162.715		21.60	D
MOTA	5341	C	GLY		16		57.194		163.780		20.80	D
ATOM	5342	0	GLY		16		58.195		164.467		23.81	D
MOTA	5343	N	SER		17		56.385		163.973		17.38	D
MOTA	5344	CA	SER		17		56.755		164.968		15.97	D
MOTA	5345	CB	SER	D	17		57.572	70.425	164.303	1.00	22.87	D

MOTA	5346	OG	SER	D	17	56.748	71.269	163.514	1.00	30.46	D
MOTA	5347	C	SER	D	17	55.581	69.927	165.691	1.00	14.56	D
MOTA	5348	0	SER	D	17	54.463	69.931	165.177	1.00	14.95	D
ATOM	5349	N	ALA	D	18	55.830	70.452	166.888	1.00	13.49	D
MOTA	5350	CA	ALA	D	18	54.764	71.078	167.657	1.00	14.66	D
ATOM	5351	CB	ALA	D	18	54.017	70.041	168.466	1.00	13.05	D
MOTA	5352	С	ALA	D	18	55.284	72.144	168.579	1.00	22.81	D
ATOM	5353	0	ALA	D	18	56.458	72.149	168.960	1.00	29.79	D
ATOM	5354	N	ASN	D	19	54.383	73.049	168.939	1.00	23.69	D
MOTA	5355	CA	ASN	D	19	54.685	74.139	169.842	1.00	20.68	D
ATOM	5356	CB	ASN	D	19	53.772	75.334	169.562	1.00	17.54	D
ATOM	5357	CG	ASN	D	19	54.211	76.135	168.361	1.00	16.26	D
MOTA	5358	OD1	ASN	D	19	55.198	75.797	167.706	1.00	13.52	D
ATOM	5359	ND2	ASN	D	19	53.479	77.211	168.061	1.00	6.31	D
ATOM	5360	C	ASN	D	19	54.433	73.692	171.260	1.00	22.94	D
ATOM	5361	0	ASN	D	19	53.491	72.961	171.532	1.00	25.61	D
MOTA	5362	N	VAL	D	20	55.268	74.139	172.177	1.00	26.10	D
MOTA	5363	CA	VAL	D	20	55.046	73.808	173.569	1.00	29.01	D
ATOM	5364	CB	VAL	D	20	56.117	72.866	174.082	1.00	30.34	D
MOTA	5365	CG1	VAL	D	20	55.786	72.461	175.499	1.00	36.31	D
MOTA	5366	CG2	VAL	D	20	56.179	71.651	173.185	1.00	17.55	D
MOTA	5367	C	VAL	D	20	55.078	75.128	174.330	1.00	27.78	D
ATOM	5368	0	VAL	D	20	56.125	75.754	174.430	1.00	28.94	D
MOTA	5369	N	TYR	D	21	53.926	75.543	174.846	1.00	26.42	D
MOTA	5370	CA	TYR	D	21	53.794	76.808	175.578	1.00	28.63	D
MOTA	5371	CB	TYR	D	21	52.419	77.409	175.286	1.00	22.74	D
MOTA	5372	CG	TYR	D	21	52.Ì16	77.456	173.815	1.00	27.07	D
MOTA	5373	CD1	TYR	D	21	51.297	76.508	173.226	1.00	24.22	· D
MOTA	53,74	CE1	TYR	D	21	51.046	76.526	171.850	1.00	29.42	. D
ATOM	5375	CD2	TYR	D	21	52.687	78.439	172.994	1.00	30.98	. D
MOTA	5376	CE2	TYR	D	21	52.445	78.471	171.627	1.00	29.68	D
MOTA	5377	CZ	TYR	D	21 .	51.620	77.510	171.060-	1.00	35.48	D
ATOM	5378	OH	TYR	D	21	51.339	77.546	169.714	1.00	35.61	D
MOTA	5379	C	TYR	D	21	53.999	76.690	177.096	1.00	31.93	D
MOTA	5380	. 0	TYR	D	21	53.221	76.019	177.792	1.00	34.89	D
MOTA	5381	N	VAL	D	2 2	55.020	77.377	177.610	1.00	31.86	D
MOTA	5382	CA	VAL	D	22	55.355	77.318	179.042	1.00	31.50	D
MOTA	5383	CB	VAL		22	56.776	76.822	179.262	1.00	29.55	D
ATOM	5384	CG1	VAL		22	56.952	75.463	178.647	1.00	27.42	D
MOTA	5385	CG2			22	57.745	77.823	178.690	1.00	25.10	D
ATOM	5386	С	VAL		22	55.282		179.859	1.00	30.58	D
MOTA	5387	0	VAL		22	55.792	79.628	179.434	1.00	31.73	D
MOTA	5388	N	ASN		23	54.678		181.045		30.13	D
MOTA	5389	CA	ASN		23	54.608		181.965		33.35	D
MOTA	5390	CB	ASN		23	53.389		182.841	•	34.26	D
MOTA	5391	CG	ASN		23	52.179		182.073		33.36	D
MOTA	5392		ASN		23	51.426		181.556		31.84	Ď
MOTA	5393		ASN		23	51.988		181.970		45.18	D
MOTA	5394	C	ASN		23	55.863		182.836		35.03	D
MOTA	5395	0	ASN		23	56.071		183.453		31.46	D
MOTA	5396	N	LEU		24	56.698		182.872		35.88	D
ATOM	5397	CA	LEU		24	57.942		183.645		35.56	D
ATOM	5398	CB	LEU		24	59.100		182.758		31.96	D
ATOM	5399	CG	LEU		24	59.274		181.399		26.28	D
ATOM	5400		LEU		24	59.974		180.457		18.62	D
MOTA	5401		LEU		24	60.070		181.523		26.70	D
MOTA	5402	C	LEU		24	57.908		184.888		35.50	D
MOTA	5403	0	LEU	D	24	57.108	82.331	184.965	1.00	38.67	D

MOTA	5404	N	ALA	D	25	58.771	81.106	185.861	1.00	33.58	D
MOTA	5405	CA	ALA	D	25	58.875	81.923	187.080	1.00	31.95	. D
MOTA	5406	CB	ALA		25	60.106	81.539	187.835	1.00	24.42	D
MOTA	5407	C	ALA	D	25	59.000	83.369	186.607	1.00	33.36	D
MOTA	5408	0	ALA	D	25	59.872-	83.691	185.812	1.00	39.23	D
MOTA	5409	N	PRO		26	58.149	84.261	187.095	1.00	29.18	D
MOTA	5410	CD	PRO	D	26	57.140	84.050	188.131	1.00	31.01	D
MOTA	5411	CA	PRO	D	26	58.188	85.672	186.682	1.00	33.36	. D
MOTA	5412	CB	PRO	Ð	26	56.976	86.288	187.406	1.00	34.37	D
MOTA	5413	CG	PRO	D	26	56.133	85.132	187.779	1.00	41.30	D
MOTA	5414	C	PRO	D	26	59.476	86.466	186.991	1.00	35.68	. D
MOTA	5415	0	PRO	D	26	59.792	87.443	186.300	1.00	33.16	D
ATOM	5416	N	VAL	D	27 .	60.184	86.046	188.040	1.00	34.83	D
MOTA	5417	CA	VAL	D	27	61.402	86.687	188.502	1.00	32.24	D
MOTA	5418	CB	VAL	Ď	27	61.137	87.469	189.780	1.00	34.79	D
MOTA	5419	CG1	VAL	D	27	62.437	88.011	190.338	1.00	34.21	D
ATOM	5420	CG2	VAL	D	27	60.143	88.574	189.507	1.00	34.74	D
MOTA	5421	C	VAL	D	27	62.486	85.683	188.831	1.00	33.29	D
ATOM	5422	0	VAL	D	27	62.237	84.684	189.495	1.00	36.62	D
MOTA	5423	N	VAL	D	28	63.700	85.965	188.389	1.00	33.27	D.
MOTA	5424	CA	VAL	D	28	64.824	85.087	188.660	1.00	35.23	D
MOTA	5425	CB	VAL		28	65.087	84.146	187.461	1.00	33.34	D
ATOM	5426		VAL	_	28 .	66.202	83.151	187.786	1.00	35.25	D
MOTA	5427	CG2	VAL		28	63.808		187.097	1.00	31.50	D
ATOM	5428	C	VAL	D	28	66.021	86.012	188.883	1.00	40.85	D
MOTA	5429	0	VAL		28	66.215	86.994	188.154	1.00	44.35	D
MOTA	5430	N	asn	D	29	66.826	85.710	189.895		40.68	D
MOTA	5431	CA	ASN		29	67.975		190.191	1.00	37.56	D
MOTA	5432	CB	ASN ·		29	68.204	86.652	191.694	1.00	30.21	D
ATOM.	5433	CG	ASN	D	29	67.004	87.167	192.423	1.00	33.80	, D
MOTA			ASN		29	66.495	88.237	192.117	1.00	35.33	D
MOTA	5435		asn		29 .	66.536		193.406	1.00	43.52	D
MOTA	5436	C	ASN		29	69.227		189.575	1.00	36.11	D
MOTA	5437	0	ASN		29	69.333		189.306		31.46	D
MOTA	5438	N	VAL		30	70.183		189.368		34.45	D
ATOM	5439	CA	VAL		30	71.461		188.835		35.36	D
MOTA	5440	CB	VAL		30	72.463		188.859		32.27	D
MOTA	5441		VAL		30	73.841		188.390		29.74	Ď
MOTA	5442		VAL		30	71.954		187.968		27.96	D
MOTA	5443	C	VAL		30	71.900		189.811		39.31	D
ATOM	5444	0	VAL		30	71.595		191.002	1.00	36.78	D
ATOM	5445	N	GLY		31	72.576		189.309		44.19	D
ATOM	5446	CA	GLY		31	73.031		190.185		48.84	D
ATOM	5447	C	GLY		31	72.044		190.375		50.83	D
MOTA	5448	0	GLY		31 .	72.464		190.574		52.00	D
ATOM	5449	N	GLN		32	70.744		190.316		49.73	D
MOTA	5450	CA	GLN		32	69.724		190.485		50.93	D
ATOM	5451	CB	GLN			68.430		190.983		52.59	D
MOTA	5452	CG	GLN		32	68.335		192.489		62.57	D
ATOM	5453	CD	GLN		32	67.252		192.937		67.08	D
MOTA	5454		GLN		32	66.156		192.363		66.36	D
MOTA	5455		GLN		32	67.551		193.978		68.68	D
MOTA	5456	C	GLN		32	69.431		189.220		52.33	D.
MOTA	5457	0	GLN		32	70.000		188.148		51.38	D
MOTA	5458 E4E9	N	ASN		33	68.544		189.368		49.70	D
ATOM	5459 5460	CA	ASN		33	68.155		188.266		47.04	D
MOTA MOTA	5460 5461	CB	ASN		33	68.312		188.656		40.13	D
MION	5461	CG	ASN	ע	33	69.625	10.705	188.208	1.00	46.47	D

							•	
MOTA	5462	OD1	ASN D	33	69.998	75.601 188.623	1.00 39.03	D
MOTA	5463	ND2	ASN I	33	70.335	77.424 187.344	1.00 45.09	D
MOTA	5464	C	ASN I	33	66.714	78.961 187.819	1.00 50.10	D
MOTA	5465	0	ASN I	33	65.782	79.029 188.624	1.00 52.06	D
MOTA	5466	N	LEU I	34	66.536	79.084 186.518	1.00 51.65	D
MOTA	5467	CA	LEU I	34	65.205	79.188 185.957	1.00 50.51	D
ATOM	5468	CB	LEU I	34	65.180	80.156 184.787	1.00 47.71	D
MOTA	5469	CG	LEU D	34	63.904	80.080 183.962	1.00 43.39	D
MOTA	5470	CD1	LEU D	34	62.755	80.760 184.687	1.00 37.93	D
MOTA	5471	CD2	LEU D	34	64.171	80.738 182.622	1.00 47.60	D
ATOM	5472	С	LEU D	34	65.042	77.753 185.453	1.00 50.83	D
MOTA	5473	0	LEU I	34	65.919	77.218 184.748	1.00 47.19	D
ATOM	5474	N	VAL I	35	63.949	77.113 185.830	1.00 47.27	D
MOTA	5475	CA	VAL I	35	63.773	75.744 185.407	1.00 45.72	D
MOTA	5476	CB	VAL D	35	63.626	74.823 186.627	1.00 47.91	D
MOTA	5477	CG1	VAL D	35	63.499	73.378 186.179	1.00 47.30	D
MOTA	5478	CG2	VAL I	35	64.840	74.994 187.534	1.00 42.49	D
ATOM	5479	С	VAL D	35	62.595	75.549 184.488	1.00 40.70	D
MOTA	5480	0	VAL D	35	61.467	75.913 184.825	1.00 39.68	D
ATOM	5481	N	VAL D	36	62.867	74.987 183.315	1.00 37.55	D
ATOM	5482	CA	VAL D	36	61.801	74.711 182.363	1.00 38.43	D
ATOM	5483	CB	VAL D	36	62.098	75.248 180.969	1.00 37.19	D
MOTA	5484	CG1	VAL D	36	60.791	75.497 180.256	1.00 40.67	D
ATOM	5485	CG2	VAL I	36	62.908	76.513 181.053	1.00 31.30	D.
MOTA	5486	С	VAL I	36	61.730	73.209 182.289	1.00 38.19	D
MOTA	5487	0	VAL D	36	62.590	72.559 181.688	1.00 38.88	D
MOTA	5488	N	ASP D	37	60.716	72.645 182.926	1.00 38.30	D
MOTA	5489	CA	ASP D	37	60.581	71.198 182.935	1.00 41.83	D
ATOM	5490	CB	ASP D	37	60.160	70.740 184.326	1.00 44.36	. D
ATOM	5491	CG	ASP D	37	60.215	69.249 184.478	1.00 53.50	D
ATOM	5492	OD1	ASP D	37	61.242	68.645 184.072	1.00 56.96	D
MOTA	5493	OD2	ASP D	. 37	59.230	68.685 185.006	1.00 61.91	D
MOTA	5494	C	ASP D	37	59.583	70.721 181.891	1.00 37.58	D
ATOM	5495	0	ASP D	37	58.375	70.871 182.063	1.00 40.31	D
MOTA	5496	N	LEU I	38	60.087	70.135 180.816	1.00 33.17	D
ATOM	5497	CA	LEU D	38	59.205	69.681 179.753	1.00 38.45	D
MOTA	5498	CB	LEU D	38	59.944	69.736 178.421	1.00 34.29	D
MOTA	5499	CG	LEU D	38	60.253	71.205.178.147	1.00 29.05	D
ATOM	5500	CD1	LEU I	38	61.183	71.294 177.012	1.00 37.61	D
MOTA	5501	CD2	LEU D	38	58.988	71.983 177.860	1.00 29.88	D
MOTA	5502	C	LEU D	38	58.578	68.312 179.979	1.00 39.31	D
MOTA	5503	0	LEU D	38	57.541	67.987 179.368	1.00 32.02	D
ATOM	5504	N	SER I	39	59.201	67.540 180.875	1.00 39.30	D
MOTA	5505	CA	SER I		58.735	66.204 181.245	1.00 38.41	D
MOTA	5506	CB	SER I		59.584	65.624 182.364	1.00 44.05	D
MOTA	5507	QG	SER I		59.134	66.126 183.617	1.00 44.75	D
MOTA	5508	С	SER I		57.334	66.367 181.786	1.00 35.99	D
ATOM	5509	0	SER I		56.616	65.403 182.018	1.00 37.62	D
ATOM	5510	N	THR I		56.954	67.609 182.010	1.00 32.86	D
MOTA	5511	CA	THR I		55.642	67.871 182.520	1.00 30.31	D
ATOM	5512	CB	THR I	40	55.705	69.015 183.541	1.00 27.64	D
MOTA	5513		THR I		55.288	68.509 184.808	1.00 35.55	D
MOTA	5514		THR I		54.816	70.172 183.150	1.00 21.43	D
ATOM	5515	C	THR I		54.725	68.222 181.377	1.00 30.56	D
MOTA	5516	0	THR I		53.501	68.248 181.530	1.00 31.24	D
MOTA	5517	N	GLN I		55.308	68.470 180.212	1.00 32.19	D
MOTA	5518	CA	GLN I		54.488	68.872 179.079	1.00 36,72	, D
ATOM	5519	CB	GLN I	41	54.773	70.333 178.759	1.00 42.92	D

					5						
ATOM	5520	CG	GLN	D	41	54.345	71.270	179.864	1.00	46.49	מ
ATOM	5521	CD	GLN	D	41	53.678		179.310		53.46	D
ATOM	5522	OE1	GLN	D	41	54.340		178.821		59.57	D
ATOM	5523	NE2	GLN	D	41	52.349		179.344		54.24	D
MOTA	5524	С	GLN	D	41	54.588		177.801		35.51	D.
MOTA	5525	0	GLN	D	41	53.803		176.879	1.00	31.88	D
MOTA	5526	N	ILE	ם .	42	55.545		177.742	1.00	33.84	D
ATOM	5527	CA	ILE	D .	42	55.724		176.547	1.00	32.88	Ď
MOTA	5528	СВ	ILE	D .	42	57.020	66.713	175.833	1.00	28.07	D
ATOM	5529	CG2	ILE	D .	42	57.183		174.567	1.00	34.76	D
MOTA	5530	CG1	ILE	D .	42	56.995		175.494	1.00	27.76	D
ATOM	5531	CD1	ILE	D .	42	58.309		174.960		34.03	. D
ATOM	5532	С	ILE	D .	42	55.740		176.866		36.38	D
ATOM	5533	0	ILE	D .	42	56.599	64.344	177.619	1.00	33.44	D.
ATOM	5534	N	PHE	ם .	43	54.779	64.124	176.272		38.64	D
MOTA	5535	CA	PHE	D .	43	54.617	62.685	176.462	1.00	38.64	D
ATOM	5536	CB	PHE	ָׁם כ	43	53.300	62.410	177.167	1.00	35.19	D
MOTA	5537	CG	PHE	D .	43	53.176	63.105	178.470	1.00	36.76	D
MOTA	5538	CD1	PHE	D .	43	52.732	64.421	178.528	1.00	35.03	D
ATOM	5539	CD2	PHE	D .	43	53.560	62.462	179.649	1.00	41.65	D
MOTA	5540	CE1	PHE	D .	43	52.669	65.095	179.744	1.00	36.26	D
ATOM	5541	CE2	PHE	D ·	43	53.505	63.121	180.871	1.00	40.83	D
ATOM	5542	CZ	PHE	D 4	43	53.057	64.444	180.923	1.00	37.78	D
ATOM	5543	C	PHE	D ·	43	54.665	61.850	175.196	1.00	40.30	D
ATOM	5544	0	PHE		43	54.162	62.243·	174.153	1.00	44.47	D
MOTA	5545	N	CYS		44	55.266		175.299	1.00	40.91	D
ATOM	5546	CA	CYS	-	44	55.343	59.777	174.164	1.00	42.07	D
ATOM	5547	С	CYS		44	54.956	58.352	174.601	1.00	43.01	D
ATOM	5548	0	CYS		44	54.817	58.059	175.796	1.00	43.90	. Б
MOTA	5549	CB	CYS		44	56.756	59.778	173.595	1.00	44.51	D
ATOM	5550	SG	CYS		44	57.417		173.127		48.68	D
ATOM	5551	N	HIS		45	54.768		173.628		39.90	D
MOTA	5552	CA	HIS		45	54.404		173.926		36.67	D
ATOM	5553	CB	HIS		45	52.897		174.129		30.05	D
ATOM	5554	CG	HIS		45	52.105		172.877		38.40	D
ATOM	5555		HIS		45	52.045		171.741		40.05	D
ATOM	5556		HIS		45	51.307		172.659		41.79	ם
ATOM	5557		HIS		45 45	50.796		171.442		43.93	D
MOTA	5558		HIS		45 45	51.229		170.863		41.62	ם
MOTA	5559	C	HIS		45 45	54.826		172.756		37.41	D
ATOM ATOM	5560 5561	N	HIS ASN		45 46	55.002		171.648		38.92	D
ATOM	5562	CA	ASN		46 46	54.997		173.026		39.62	D
ATOM	5563	CB	ASN		46	55.375 56.081		172.037		40.59	D
ATOM	5564	CG	ASN		46	56.831		172.755 171.815		42.61 40.31	D D
ATOM	5565		ASN		46						_
MOTA	5566		ASN		46	56.327		170.759 172.197		40.56 35.28	D
MOTA	5567	C	ASN		46	54.037		171.463		42.95	D
MOTA	5568	ō	ASN		46	53.074		172.208		42.82	D D
MOTA	5569	N	ASP		47	53.947		170.159		44.85	D
MOTA	5570	CA	ASP		47	52.670		169.602		48.92	D
MOTA	5571	CB	ASP		47	52.437		168.205		46.60	D
MOTA	5572	CG	ASP		47	51.947		168.262		48.03	D
MOTA	5573		ASP		47	50.909		168.904		49.27	D
	5574		ASP		47	52.593		167.656		47.69	D
MOTA	5575	C	ASP		47	52.563		169.547		49.01	ם
MOTA	5576	ō	ASP		47	51.469		169.560		47.25	D
ATOM	5577	N	TYR		48	53.704		169.496		48.84	D

ATOM	5578	CA	TYR I	D 48	53.718	48.132 169.452	1.00 48.99	D
MOTA	5579	CB	TYR :		53.971	47.651 168.024	1.00 51.60	D
MOTA	5580	CG	TYR :	D 48	53.001	48.240 167.015	1.00 57.36	D
ATOM	5581	CD1	TYR :	D 48	53.330	49.396 166.298	1.00 60.60	D
MOTA	5582	CEl	TYR :	D 48	52.435	49.968 165.396	1.00 61.32	D
MOTA	5583	CD2	TYR :	D 48	51.742	47.665 166.800	1.00 57.87	, D
MOTA	5584	CE2	TYR I	D 48	50.833	48.233 165.899	1.00 60.38	D
MOTA	5585	CZ	TYR I	D 48	51.190	49.388 165.205	1.00 61.77	D
MOTA	5586	OH	TYR I	D 48	50.298	49.994 164.354	1.00 59.47	D
MOTA	5587	C	TYR I	D 48	54.800	47.634 170.393	1.00 48.38	D
ATOM	5588	0	TYR I	D 48	55.802	47.055 169.964	1.00 49.69	D
MOTA	5589	N	PRO 1	D 49	54.600	47.856 171.701	1.00 47.71	D
MOTA	5590	CD	PRO 1	D 49	53.397	48.476 172.283	1.00 49.30	D
ATOM	5591	CA	PRO 1	D 49	55.535	47.454 172.753	1.00 50.81	D
MOTA	5592	CB	PRO 1	D 49	54.788	47.821 174.040	1.00 49.19	D
MOTA	5593	CG	PRO I	D 49	53.348	47.848 173.634	1.00 47.87	D
ATOM	5594	C	PRO I	D 49	55.991	45.997 172.719	1.00 54.81	D
ATOM	5595	0	PRO I	D 49	57.189	45.727 172.621	1.00 55.51	D
MOTA	5596	N	GLU I	D 50	55.036	45.067 172.780	1.00 56.17	D
MOTA	5597	CA	GLU I	D 50	55.318	43.623 172.777	1.00 54.59	D
MOTA	5598	CB	GLU I	D 50	54.025	42.817 172.631	1.00 47.73	D
MOTA	5599	CG	GLU I	D 50	52.923	43.186 173.595	1.00 55.13	D
MOTA	5600	CD	GLU 1	D 50	52.230	44.484 173.218	1.00 63.88	D
ATOM	5601	OE1	GLU I	D 50	52.407	44.948 172.061	1.00 63.40	D
MOTA	5602	OE2	GLU 1	D 50	51.497	45.033 174.073	1.00 63.47	D
MOTA	5603	C	GLU I	D 50	56.302	43.090 171.732	1.00 53.44	D
ATOM	5604	0	GLU 1	D 50	56.875	42.023 171.925	1.00 56.75	D
ATOM	5605	N	THR I	D 51	56.507	43.803 170.632	1.00 48.96	D
MOTA	5606	CA	THR I	D 51	57.415	43.295 169.608	1.00 52.60	D
ATOM	5607	CB	THR I	D 51	56.612	42.792 168.376	1.00 53.57	D
MOTA	5608	OG1	THR I	D 51	56.331	43.879 167.477	1.00 46.96	. D
MOTA	5609	CG2	THR 1	D 51	55.290	42.219 168.840	1.00 55.69	D
ATOM	5610	C	THR I	D 51	58.437	44.339 169.156	1.00 55.47	D
MOTA	5611	0	THR I	D 51	59.407	44.025 168.452	1.00 55.82	D
MOTA	5612	N	ILE 1	D 52	58.225	45.586 169.558	1.00 51.66	D
MOTA	5613	CA	ILE I	D 52	59.145	46.627 169.163	1.00 45.39	D
MOTA	5614	CB	ILE I	D 52	58.512	47.541 168.116	1.00 49.25	D
MOTA	5615	CG2	ILE I	D 52	59.467	48.670 167.755	1.00 46.46	D
MOTA	5616	CG1	ILE :	D 52	58.150	46.717 166.875	1.00 48.34	D
MOTA	5617	CD1	ILE 1	D 52	57.480	47.514 165.783	1.00 50.24	D
MOTA	5618	C	ILE 1	D 52	59.561	47.453 170.347	1.00 44.62	D
MOTA	5619	0	ILE I		58.744	47.774 171.205	1.00 42.27	D
MOTA	5620	N	THR 1		60.851	47.762 170.407	1.00 45.97	D
MOTA	5621	CA	THR I		61.385	48.593 171.475	1.00 48.38	D
ATOM	5622	CB	THR I		62.564	47.910 172.195	1.00 50.53	D
MOTA	5623	OG1	THR I		62.052	46.994 173.176	1.00 48.05	D
ATOM	5624	CG2			63.447	48.948 172.885	1.00 47.27	D
ATOM	5625	C	THR I		61.839	49.917 170.877	1.00 48.03	D
MOTA	5626	0	THR I		62.657	49.942 169.947	1.00 44.73	D
MOTA	5627	N	ASP I		61.293	51.011 171.413	1.00 50.05	D
ATOM	5628	CA	ASP 1		61.616	52.354 170.931	1.00 49.86	D
MOTA	5629	CB	ASP I	D 54	60.355	53.232 170.937	1.00 48.25	D
MOTA	5630	CG	ASP 1	D 54	59.374	52.870 169.821	1.00 46.20	D
MOTA	5631		ASP !		59.837	52.582 168.698	1.00 48.29	D
MOTA	5632		ASP 1		58.145	52.890 170.057	1.00 42.24	D
MOTA	5633	С	ASP 1		62.733	53.047 171.721	1.00 47.79	D
ATOM	5634	0	ASP I		62.809	52.936 172.946	1.00 43.23	D
MOTA	5635	N	TYR :	D 55	63.595	53.756 170.990	1.00 50.75	D

MOTA	5636	CA	TYR D	55	64.730	54.502 171.554	1.00 51.63	D
ATOM	5637	CB	TYR D	55	66.036	54.057 170.899	1.00 52.94	D
MOTA	5638	CG	TYR D	55	66.308	52.580 170.991	1.00 53.68	D
MOTA	5639	CD1	TYR D	55	66.715	51.869 169.858	1.00 51.76	D
MOTA	5640	CE1	TYR D	55	66.948	50.507 169.908	1.00 51.50	D
MOTA	5641	CD2	TYR D	55	66.146	51.887 172.197	1.00 50.68	D
MOTA	5642	CE2	TYR D	55	66.380	50.514 172.265	1.00 55.22	D
ATOM	5643	CZ	TYR D	55	66.779	49.829 171.107	1.00 54.89	D
MOTA	5644	OH	TYR D	55	66.986	48.469 171.129	1.00 49.34	D
MOTA	5645	C	TYR D	55	64.581	56.009 171.325	1.00 48.85	D
MOTA	5646	0	TYR D	55	64.646	56.483 170.190	1.00 48.91	D
MOTA	5647	N	VAL D	56	64.396	56.752 172.409	1.00 47.81	D
MOTA	5648	CA	VAL D	56	64.241	58.198 172.338	1.00 45.40	D
MOTA	5649	CB	VAL D	56	63.075	58.650 173.192	1.00 43.96	D
MOTA	5650	CG1	VAL D	56	62.973	60.164 173.169	1.00 48.40	D
MOTA	5651	CG2	VAL D	56	61.811	58.021 172.664	1.00 45.38	D
MOTA	5652	С	VAL D	56	65.50 6	58.908 172.790	1.00 44.94	D
MOTA	5653	0	VAL D	56	66.077	58.607 173.823	1.00 47.71	D
ATOM	5654	N	THR D	57	65.915	59.897 172.021	1.00 46.85	D
MOTA	5655	CA	THR D	57	67.150	60.612 172.292	1.00 41.59	D
MOTA	5656	CB	THR D	57	68.178	60.122 171.271	1.00 33.45	D
MOTA	5657		THR D	57	69.478	60.114 171.836	1.00 37.75	. D
MOTA	5658	CG2	THR D	57	68.159	61.001 170.067	1.00 24.52	Q
MOTA	5659	C	THR D	57	66.968	62.135 172.139	1.00 41.37	D
ATOM	5660	.0	THR D	57	66.090	62.570 171.394	1.00 43.18	D
ATOM	5661	N	LEU D	58	67.773	62.938 172.841	1.00 38.63	D
ATOM	5662	CA	LEU D	58	67.698	64.393 172.680	1.00 38.82	D
MOTA	5663	CB	LEU D	58	68.012	65.135 173.981	1.00 38.58	· D
ATOM -	5664	CG	LEU D	58	68.130	66.662 173.793	1.00 40.37	D
ATOM	5665		LEU D	. 58	66.765	67.237 173.408	1.00 37.66	D
MOTA	5666	CD2	-	58	68.643	67.332 175.053	1.00 33.86	, D
ATOM	5667	G.	LEU D	58	68.735	64.785 171.619	1.00 41.06	. D
ATOM	5668	0	LEU D	58	69.847	65.228 171.945	1.00 43.92	D
ATOM	5669	N	GLN D	59	68.350	64.610 170.356	1.00 40.77	D
ATOM	5670	CA	GLN D	59	69.179	64.900 169.181	1.00 40.87	D
ATOM	5671	CB	GLN D	59	68.291	64.870 167.933	1.00 46.84	D
MOTA	5672	CG	GLN D	59	68.800	64.053 166.754	1.00 58.79	D
ATOM	5673 5674	CD	GLN D	59	70.198	64.427 166.328	1.00 68.42	D
ATOM	5675		GLN D	59	71.183	63.989 166.927	1.00 77.06	D
ATOM ATOM	5676	NE2 C	GLN D	59 59	70.299	65.250 165.290	1.00 74.25	D
ATOM	5677	o	GLN D	59	69.918 71.114	66.247 169.226	1.00 38.61 1.00 35.55	D
ATOM	5678	N	ARG D	60	69.187	66.317 168.953 67.308 169.559		D
ATOM	5679	CA	ARG D	60	69.741	68.651 169.618	1.00 36.04 1.00 36.19	D D
MOTA	5680	CB	ARG D	60	69.805	69.229 168.199	1.00 37.08	D
ATOM	5681	CG	ARG D	60	. 70.596	70.520 168.047	1.00 47.03	
ATOM	5682	CD	ARG D	60	70.500	71.078 166.621	1.00 56.12	. D
ATOM	5683	NE	ARG D	60	70.137	70.049 165.637	1.00 72.98	. D
ATOM	5684	CZ	ARG D	60	70.899	69.003 165.292	1.00 77.04	D
ATOM	5685		ARG D	60	72.098	68.821 165.843	1.00 76.99	D
ATOM	5686		ARG D	60	70.453	68.121 164.399	1.00 73.66	D
ATOM	5687	C	ARG D	60	68.887	69.552 170.519	1.00 36.39	D
ATOM	5688	ō	ARG D	60	67.696	69.320 170.698	1.00 43.92	D
ATOM	5689	N	GLY D	61	69.506	70.573 171.092	1.00 33.53	D
ATOM	5690	CA	GLY D	61	68.804	71.503 171.954	1.00 31.15	D
ATOM	5691	C	GLY D	61	69.350	72.865 171.592	1.00 31.13	D
ATOM	5692	Ō	GLY D	61	70.561	73.062 171.608	1.00 34.33	D
ATOM	5693	N	SER D	62	68.471	73.805 171.260	1.00 34.12	D
						- · · · · · · · · · · · · · · · · · · ·		

MOTA	5694	CA	SER	D	62	68.920	75.122	170.852	1.00	33.13	D
ATOM	5695	CB	SER	ם	62	68.759	75.270	169.341	1.00	34.81	D
MOTA	5696	OG	SER	D	62	69.546	74.312	168.661	1.00	33.21	D
ATOM	5697	С	SER	D	62	68.189		171.542	_	35.12	D
MOTA	5698	0	SER	D	62	66.986		171.778	_	40.21	D
ATOM	5699	N	ALA	D	63	68.924		171.825	_	34.52	D
ATOM	5700	CA	ALA		63	68.384		172.514		29.48	D
ATOM	5701	CB	ALA		63	69.369		173.563		29.03	D
ATOM	5702	C	ALA		63	68.058		171.564			
ATOM	5703	ō	ALA		63	68.665		170.520		26.39	D
ATOM	5704	Ŋ	TYR							29.01	D
ATOM		_		_	64	67.098		171.948		25.45	ם
MOTA	5705	CA	TYR		64 .	66.668		171.141		25.29	D
	5706	CB	TYR		64	65.439		170.296		29.09	D
ATOM	5707	CG	TYR		64	65.740		169.244		34.22	D
ATOM	5708	CD1			64	65.695		169.540		37.16	D
MOTA	5709	CE1			64	66.087		168.599		40.42	D
ATOM	5710	CD2	TYR		64	66.171		167.984	1.00	34.69	D
MOTA	5711	CE2			64	66.562		167.045	1.00	35.37	D
MOTA	5712	CZ	TYR		64	66.523		167.352	1.00	42.68	D
MOTA	5713	OH	TYR		64	66.941		166.413	1.00	52.45	D
MOTA	5714	C	TYR	D	64	66.336	82.792	171.997	1.00	26.55	D
ATOM	5715	0	TYR	D	64	66.082	82.662	173.199	1.00	30.08	D
MOTA	5716	N	GLY		65	66.339	83.963	171.365	1.00	24.96	D
MOTA	5717	CA	GLY	D	65	66.036	85.197	172.060	1.00	24.91	D
MOTA	5718	C	GLY.	D	65	66.800	85.352	173.358	1.00	28.86	D
MOTA	5719	0	GLY	D	65	68.014	85.060	173.445	1.00	28.91	D
ATOM	5720	N	GLY	D	66	66.075	85.792	174.381	1.00	25.34	D
ATOM	5721	CA	GLY	D	66	66.683	86.018	175.674	1.00	27.04	D
ATOM	5722	С	GLY	D	66	67.464		176.183		26.29	D
MOTA	5723	ο .	GLY	D	66	68.574	84.998	176.636		32.30	D
ATOM	5724	N	VAL	D	67	66.889	83.653	176.112		27.48	D
ATOM	5725	CA	VAL	D	67	67.585		176.599		30.59	D
MOTA	5726	CB	VAL		67	66.864		176.189		28.05	D
ATOM	5727	CG1	VAL	D	67	67.796		176.374		23.61	D
ATOM	5728		VAL		67	65.605		177.034		18.84	Ď
ATOM	5729	C	VAL		67	69.009		176.083		34.05	D
ATOM	5730	ō	VAL		67	69.932		176.803		36.67	D
ATOM	5731	N	LEU		68	69.169		174.831	_	36.19	D
ATOM	5732	CA	LEU		68	70.454		174.155		38.03	D
ATOM	5733	CB	LEU		68	70.189		172.663		38.26	D
ATOM	5734	CG	LEU		68	71.270		171.633		32.92	D
ATOM	5735		LEU		68	71.832		171.803		26.29	D
ATOM	5736		LEU		68	70.642		170.256		29.24	D
ATOM	5737	C	LEU		68	71.432	•	174.584		40.10	
ATOM	5738	Ö	LEU		68	72.642		174.564		41.49	D
ATOM	5739	И	SER		69	70.911		174.8877			D
MOTA	5740	CA	SER		69	71.784				38.23 · 38.34	D
MOTA	5741	CB	SER		69	71.764		175.237			D
ATOM		OG	SER		69			174.560		37.73	D
ATOM	5742					69.954		174.938		34.57	D
	5743	C	SER		69	71.955		176.716		37.45	D
MOTA	5744	0	SER		69	72.970		177.113		36.78	D
MOTA	5745	N	ASN		70	70.977		177.526		35.91	D
MOTA	5746	CA	ASN		70	71.008		178.962		35.34	D
MOTA	5747	CB	ASN		70	69.714		179.377		34.25	D
MOTA	5748	CG	ASN		70	69.423		178.525		38.04	D
ATOM	5749		ASN		70	70.343		178.063		46.18	D
ATOM	5750		ASN		70	68.147		178.318		44.74	D
MOTA	5751	С	ASN	D	70	71.237	85.085	179.897	1.00	38.20	D

MOTA	5752	0	ASN	D	70	71.270	85.265	181.118	1.00	42.79	D
MOTA	5753	N	PHE	D	71	71.407	83.889	179.360	1.00	36.65	D
ATOM	5754	CA	PHE	D	71	71.577	82.755	180.245	1.00	33.92	D
MOTA	5755	CB	PHE	D	71	70.283	81.941	180.307	1.00	28.49	D
MOTA	5756	CG	PHE	D	71	69.114	82.681	180.876		25.93	D
MOTA	5757	CD1	PHE	D	71	68.430	83,626	180.121		30.86	D
MOTA	5758		PHE		71	68.683		182,179		20.33	D
ATOM	5759		PHE		71	67.310		180.675		39.06	D
ATOM	5760		PHE		71	67.585		182.735		22.00	D
ATOM	5761	CZ	PHE		71	66.893		181.988		24.40	D
ATOM	5762	c	PHE		71	72.701		179.857		36.97	. D
ATOM	5763	Ō	PHE		71	73.218		178.731		36.04	D
ATOM	5764	N	SER		72	73.084		180.822		35.89	D
ATOM	5765	CA	SER		72	74.091		180.613		41.93	D
ATOM	5766	CB	SER		72	75.382		181.389		43.25	D
ATOM	5767	OG	SER		72	75.176		182.787		51.92	D
ATOM	5768	C	SER		72	73.354		181.220		42.70	D
ATOM	5769	ŏ	SER		72	72.686		182.248		44.36	Ď
ATOM	5770	N	GLY		73	73.422		180.602		42.36	Ď
ATOM	5771	CA	GLY		73	72.669		181.213		43.37	D
ATOM	5772	C	GLY		73	72.949		180.797		41.31	. D
ATOM	5773	ŏ	GLY		73	73.766		179.908		37.82	Ď
MOTA	5774	N	THR		7 4 .	72.245		181.467		40.50	. D
ATOM	5775	CA	THR		74. 74	72.396		181.180		45.58	. D
ATOM	5776	CB	THR		74	73.000		182.386		47.49	D
ATOM	5777		THR		74	72.059		183.467		51.70	D
ATOM	5778	CG2			74 74	74.317		182.846		38.61	D
ATOM	5779	C	THR		74 74	71.050		180.852		42.69	
ATOM	5780	ō	THR		74 74	69.998		181.087		35.56	D
ATOM	5781	N	VAL		75 75	71.106		180.275			D
ATOM	5782	CA	VAL		75 75	69.900		179.941		44.17	D C
ATOM	5783	CB	VAL		75 75	69.753		178.396		44.78	D.
ATOM	5784		VAL		75 75	70.974		177.841		44.61	D
ATOM	5785		VAL		75 75			178.128		43.76.	D
ATOM	5786	C	VAL		75 75	68.481 70.007		180.676		33.87	D
ATOM	5787	0	VAL		75 75	71.003				43.56	D
ATOM	5788							180.539		37.52	D
ATOM		N CA	LYS LYS		76 76	69.002		181.491		43.49	. D
ATOM	5789 5790		LYS		76 76	68.990		182.220		48.22	D
		CB	LYS			68.468		183.645		52.15	D
ATOM ATOM	5791 5792	CD	LYS		76 76	68.795		184.569		59.05	D
ATOM	5793	CE	LYS		76	68.332 68.776		186.003 186.913		65.92 68.75	D
ATOM	5794	NZ	LYS		76 76	68.367	_	188.337			D
ATOM	579 5	C	LYS		76 76	68.098		181.480		72.96	D
ATOM	5796		LYS		76 76					50.18	D
	5797	N O	TYR			66.868		181.500		50.92	D
MOTA MOTA	5798				77 77	68.724				47.77	D
ATOM	5799	CA	TYR		77	67.984 68.514		180.093 178.676		46.46	D
		CB	TYR		77 77					38.80	D
MOTA	5800 5801	CG	TYR		77 77	67.678		177.868		42.71	D
MOTA			TYR		7 7	66.305		177.735		40.46	D
MOTA	5802		TYR		77 77	65.536		176.949		43.60	D
ATOM	5803		TYR		77	68.260		177.198		42.40	D
MOTA	5804	CE2			77 77	67.500		176.403		34.47	D
MOTA	5805	CZ	TYR		77	66.135		176.277		44.63	D
MOTA	5806	OH	TYR		77	65.363		175.431		45.13	D .
MOTA	5807	G ·	TYR		77 	68.036		180.733		50.05	D
MOTA	5808	0	TYR		77	69.043		180.608		51.74	D
MOTA	5809	Ŋ	SER	ע	78	66.956	62.695	181.396	1.00	52.61	D

MOTA	5810	CA	SER	D	78	66.904	61.368	181.996	1.00	55.05	D
MOTA	5811	CB	SER	D	78	67.067	60.303	180.889	1.00	54.80	D
MOTA	5812	OG	SER	D	78	66.889	58.971	181.359	1.00	52.93	D
ATOM	5813	C	SER	D	78	67.972	61.172	183.063	1.00	58.11	D
ATOM	5814	0	SER	D	78	68.764	60.236	182.990	1.00	62.64	D
MOTA	5815	N	GLY	D	79	68.013	62.059	184.047	1.00	59.15	D
MOTA	5816	CA	GLY	D	79	69.001	61.898	185.100	1.00	61.56	D
MOTA	5817	C	GLY	D	79	70.366	62.536	184.901	1.00	62.86	D
MOTA	5818	0	GLY	D	79	71.004	62.903	185.886	1.00	65.64	a
MOTA	5819	N	SER	D	80	70.825	62.665	183.656	1.00	61.18	D
MOTA	5820	CA	SER	D	80	72.128	63.281	183.378	1.00	60.35	D
MOTA	5821	CB	SER	D	80	72.915	62.431	182.389	1.00	57.76	D
MOTA	5822	OG	SER	D	80	73.236	61.193	182.977	1.00	66.01	D
MOTA	5823	C	SER	D	80	72.022	64.708	182.834	1.00	59.17	D
MOTA	5824	0	SER	D	80	70.971	65.112	182.335	1.00	58.18	D
ATOM	5825	N	SER	D	81	73.115	65.467	182.929	1.00	56.61	D
ATOM	5826	CA	SER	D	81	73.119	66.848	182.450	1.00	50.07	D
MOTA	5827	CB	SER	D	81	73.371	67.836	183.598	1.00	51.95	D
ATOM	5828	OG.	SER	D	81	72.155	68.372	184.107	1.00	47.34	D
MOTA	5829	C .	SER	D	81 .	74.120	67.088	181.344	1.00	46.16	D
MOTA	5830	0	SER	D	81	75.148	66.432	181.247	1.00	41.56	D
MOTA	5831	N	TYR	D	82	73.793	68.036	180.485	1.00	48.76	D
ATOM	5832	CA	TYR		82	74.655	68.351	179.363	1.00	49.74	D
MOTA	5833	CB	TYR	D	82	74.222	67.575	178.099	1.00	50.52	ď
MOTA	5834	CG	TYR	D	82	73.962	66.098	178.315	1.00	51.28	Ð
MOTA	5835	CD1	TYR		82	72.837	65.661	179.022	1.00	49.16	D
MOTA	5836	CE1			82	72.626	64.310	179.286	1.00	53.58	D
MOTA	5837	CD2			82	74.867		177.864	1.00	55.30	D
ATOM	5838	CE2	TYR	D	82	74.664	63.767	178.117	1.00	52.76	D
ATOM	583,9	CZ	TYR	D.	82	73.544	63.362	178.831	1.00	57.08	D
MOTA	5840	HO	TYR	D	82	73.340	62.017	179.096	1.00	59.70	D
MOTA	5841	C	TYR	D	82	74.565	69.846	179.101		47.56	D
MOTA	5842	0	TYR		82	73.615	70.528	179.525	1.00	47.60	D
MOTA	5843	N	PRO		83	75.558		178.395	1.00	42.33	D
MOTA	5844	CD	PRO		83	76.766		177.968		37.7 7	D
MOTA	5845	CA	PRO		83	75.634		178.049		42.94	. D
MOTA	5846	CB	PRO		83	76.981		177.347	1.00	39.08	D
MOTA	5847	CG	PRO		83	77.759		177.929		43.25	D
ATOM	5848	C	PRO		83	74.489		177.132		44.94	D
MOTA	5849	0	PRO		83	74.215		176.141		48.59	D
ATOM	5850	N	PHE		84	73.819		177.466		44.30	D
MOTA	5851	CA	PHE		84	72.733		176.630		44.32	D
ATOM	5852	CB	PHE		84	71.386		177.342		42.78	ם
MOTA	5853	CG	PHE		84	70.231		176.562		39.68	D
ATOM	5854		PHE		84	69.666		175.515		38.18	D
MOTA	5855		PHE		84	69.714		176.872		38.62	D
ATOM	5856		PHE		84	68.605		174.793		42.76	D
ATOM	5857		PHE		84	68.652		176.152		37.07	D
ATOM	5858	cz	PHE		84	68.096		175.115		35.45	D
MOTA	5859	C	PHE		84	72.992		176.306		46.00	D
MOTA	5860	0	PHE		84	73.184		177.213		48.06	D
MOTA	5861	И	PRO		85	72.967		175.011		45.37	D
MOTA	5862	CD	PRO		85	73.201		174.655		43.57	D
ATOM	5863	CA	PRO		85	72.737		173.800		43.76	D
ATOM ·	5864	CB	PRO		85	73.202		172.699		39.35	D
MOTA .	5865	CG	PRO		85	72.733		173.210		42.33	D
MOTA MOTA	5866	C	PRO		85	73.502		173.819		43.70	D
WIOM	5867	0	PRO	U	85	74.603	13.434	174.350	1.00	48.50	D

ATOM	5868	N	THR I	86	72.924	72.502 173.247	1.00 40.19	D
ATOM	5869	CA	THR I	86	73.575	71.202 173.247	1.00 40.13	. D
MOTA	5870	CB	THR I	86	72.585	70.096 172.924	1.00 36.77	D
ATOM	5871	OG1	THR I	8,6	72.165	70.212 171.560	1.00 38.01	D
MOTA	5872	CG2	THR I	86	71.389	70.193 173.832	1.00 36.13	D
ATOM	5873	C	THR I	86	74.706	71.147 172.241	1.00 44.65	D
MOTA	5874	0	THR I		74.745	71.933 171.299	1.00 45.24	D
ATOM	5875	N	THR I	87	75.619	70.201 172.440	1.00 50.30	ם
ATOM	5876	CA	THR I	87	76.779	70.044 171.553	1.00 53.99	D
MOTA	587 7	CB	THR I	87	78.075	70.379 172.296	1.00 53.50	D
ATOM	5878	OG1	THR I		78.015	69.825 173.619	1.00 60.15	D
MOTA	5879	CG2	THR I	87	78.265	71.872 172.377	1.00 54.91	D
MOTA	5880	С	THR I	87	76.938	68.641 170.967	1.00 55.08	D
ATOM	5881	0	THR I	87	77.770	68.430 170.091	1.00 52.17	D
ATOM	5882	N	SER I	88	76.141	67.692 171.457	1.00 57.20	D
MOTA	5883	CA	SER I		76.193	66.312 170.988	1.00 55.61	D
MOTA	5884	CB	SER I	88,	77.238	65.528 171.787	1.00 57.14	D
MOTA	5885	OG	SER I	88	76.783	65.270 173.108	1.00 56.47	D
MOTA	5886	С	SER I		74.839	65.634 171.166	1.00 54.36	D
MOTA	5887	0	SER I	88	74.034	66.053 171.996	1.00 50.10	D
ATOM	5888	N	GLU I		74.587	64.588 170.382	1.00 55.43	D
MOTA	5889	CA	GLU I		73.340	63.856 170.523	1.00 52.86	D
MOTA	5890	CB	GLU I		73.093	62.907 169.348	1.00 53.88	D
MOTA	5891	CG	GLU I		72.063	61.822 169.666	1.00 51.32	D
ATOM	5892	CD	GLU I		71.461	61.186 168.432	1.00 53.86	D
MOTA	5893		GLU D		72.194	60.925 167.457	1.00 56.99	D
ATOM	5894		GLU D		70.246	60.932 168.444	1.00 53.32	D
ATOM	5895	C	GLU D		73.471	63.063 171.810	1.00 50.22	D
MOTA	5896	0	GLU D		74.441	62.346 172.027	1.00 51.19	D
	5897	N	THR D		72.472	63.214 172.656	1.00 48.83	D
MOTA	5898	CA	THR D		72.413	62.578 173.952	1.00 46.67	D
MOTA	5899	CB	THR D		71.230	63.159 174.715	1.00 46.49	D
ATOM	5900		THR D		71.625	63.440 176.056	1.00 52.22	. D
ATOM	5901	CG2			70.055	62.201 174.694	1.00 36.21	D
ATOM	5902	C	THR D		72.278	61.061 173.895	1.00 46.92	D
ATOM	5903	0	THR D		72.067	60.494 172.836	1.00 46.69	D
ATOM	5904	N	PRO D		72.439	60.382 175.044	1.00 51.57	D
MOTA	5905	CD	PRO D		73.078	60.888 176.273	1.00 53.12	_
ATOM	5906	CA	PRO D		72.315	58.919 175.099	1.00 52.16	D
ATOM	5907	CB	PRO D		72.819	58.587 176.505	1.00 52.22	D
ATOM	5908 5909	CG C	PRO D		73.813 70.838	59.670 176.774	1.00 50.27	D
ATOM ATOM	5919 5910	0	PRO D			58.567 174.907	1.00 49.74	D
ATOM	5911	N	ARG I		69.976 70.542	59.420 175.104	1.00 50.75	D
ATOM	5912	CA	ARG D		69.154	57.319 174.553 56.914 174.308	1.00 50.26	D
ATOM	5913	CB	ARG D		69.088		1.00 52.79 1.00 55.32	D
ATOM	5914	CG	ARG D		69.893	55.979 173.087 54.691 173.189	1.00 53.32	D
ATOM	5915	CD	ARG D		69.619	53.766 171.989	1.00 62.37	D D
ATOM	5916	NE	ARG D		70.121	52.393 172.157	1.00 69.97	D
ATOM	5917	CZ	ARG D		70.018	51.666 173.275	1.00 70.74	D
ATOM	5918		ARG D		69.440	52.168 174.363	1.00 70.74	
ATOM	5919		ARG D		70.468	50.417 173.299	1.00 71.05	Ď
ATOM	5920	C	ARG D		68.357	56.289 175.454	1.00 57.34	Ď
ATOM	5921	Ö	ARG I		68.839	55.396 176.137	1.00 50.32	ם
ATOM	5922	N	VAL I		67.134	56.786 175.651	1.00 37.68	D
ATOM	5923	CA	VAL D		66.205	56.291 176.666	1.00 43.49	D
ATOM	5924	CB	VAL D		65.383	57.419 177.288	1.00 35.02	D
ATOM	5925		VAL D		64.375	56.853 178.259	1.00 34.17	D
					04.575	20.000 1/0.200	~ 34.T/	ט

					-				•	
MOTA	5926		VAL		93	66.28	 3 177.98		46.18	D
MOTA	5927	C	VAL		93	65.22	6 175.93		41.91	D
MOTA	5928	0	VAL		93	64.96	2 174.74		44.04	D
ATOM	5929	N	VAL		94	64.67	5 176.62		41.51	D
ATOM	5930		VAL		94	63.74	 7 175.93		40.64	D
MOTA	5931	CB	VAL	D	94	64.11	0 176.03		37.90	D
ATOM	5932		VAL		94	65.63	7 175.89		35.27	D
MOTA	5933		VAL		94	63.57	9 177.31		28.24	D
MOTA	5934	C	VAL		94	62.29	4 176.37		41.96	D
MOTA	5935	0	VAL		94	61.99	8 177.55		37.16	D
MOTA	5936	N	TYR		95		8 175.38		45.24	D
ATOM	5937	CA	TYR		95	59.98	1 175.57		44.43	D
ATOM	5938	CB	TYR		95	59.38	5 174.70		41.75	D
MOTA	593 9	CG	TYR		95	59.60	3 175.29		38.12	D
MOTA	5940		TYR		95	60.86	 9 175.32		32.37	D
ATOM	5941		TYR		95	61.08	8 175.95		27.99	D
MOTA	5942	CD2	TYR		95	58.55	8 175.90		40.50	D
MOTA	5943	CE2	TYR		95	58.76	4 176.54		37.43	D
ATOM	5944	CZ	TYR		95	60.04	4 176.56		39.02	D
MOTA	5945	OH	TYR		95	60.28	7 177.23		49.00	D
ATOM	5946	C	TYR		95	59.42	3 175.15		45.02	D
ATOM	5947	0	TYR		95	59.64	2 174.02		45.31	D
MOTA	5948	N	ASN		96	58.72	3 176.09		39.92	D
ATOM	5949	CA	ASN		96	58.12	0 175.87		34.46	D
MOTA	5950	CB	ASN		96	59.00	0 176.45		34.45	D
MOTA	5951	CG .	ASN		96	59.68	6 177.70		41.54	D
MOTA	5952		ASN		96	60.87	9 177.67		53.18	D
MOTA	5953		ASN		96	58.94	5 178.81		41.57	Ď
MOTA	5954	C	ASN		96	56.76	5 176.51		35.83	D
MOTA	5955	0	ASN		96	56.54	5 177.39		38.84	. D
MOTA	5956	N	SER		97	55.83	6 176.07		34.76	D
MOTA	5957	CA	SER		97	54.50	2 176.62		33.17	D
ATOM	5958	CB	SER		97	54.51	9 178.10		20.43	D
MOTA	5959	OG	SER		97	53.21	0 178.51		24.85	D
ATOM	5960	C	SER		97	53.59	8 175.83		35.40	D
ATOM	5961	0	SER		97	54.01	0 175.38		35.61	D
ATOM	5962	N	ARG		98	52.35	4 175.63		39.41	D
ATOM	5963	CA	ARG		98	51.39	5 174.90		39.57	D
ATOM	5964	CB	ARG		98	50.16 50.43	4 174.51		43.38	D
ATOM ATOM	5965 5966	CD	ARG ARG		98 98	49.12	5 173.47 1 172.92		51.67 58.46	D
ATOM	5967					49.35			-	D
ATOM	5968	NE CZ	ARG ARG		98 98	49.88	5 171.83		64.42	D
ATOM	5969		ARG		98	50.23	2 171.98 5 172 10		69.22	Ď
ATOM	5970		ARG		98	50.23	5 173.19 4 170.92		68.11 72.50	D D
ATOM	5971	C	ARG		98	50.99	 7 175.83		40.32	ם
ATOM	5972	Ö	ARG		98	50.35	 4 175.42		44.21	_
ATOM	5973	N	THR		99	51.38	1 177.09		43.11	D D
ATOM	5974	CA	THR		99	51.05	4 178.06		48.49	D
ATOM	5975	CB	THR		99	51.19	6 179.49		47.77	D
ATOM	5976		THR		99	50.50	7 179.60		49.42	. D
ATOM	5977		THR		99	50.59	1 180.46		46.69	D
ATOM	5978	C	THR		99	51.97	0 177.92		50.98	D
ATOM	5979	0	THR		99	53.20	0 177.92 0 177.86		50.95	D
ATOM	5980	N	ASP			51.37	8 177.86		50.03	D
	5981	CA	ASP			52.14	7 177.72		51.36	D
ATOM	5982	CB	ASP			51.23	1 177.63		54.66	D
ATOM	5983	CG	ASP			50.65	9 176.24		59.85	D
LIT OLI		-0	730 E	_	-00	20.03	 J 110.29	T.00	دن. در	<i>-</i>

MOTA	5984	OD1	ASP I	100	51.330	58.949	175.249	1.00 59.61	D
MOTA	5985	OD2	ASP I	1.00	49.518	59.810	176.165	1.00 57.94	D
MOTA	5986	C	ASP I		53.099		178.879	1.00 50.93	D
ATOM	5987	0	ASP I		52.684		180.000	1.00 49.74	D
ATOM	5988	N	LYS I		54.386	58.002	178.578	1.00 53.17	D.
ATOM	5989	CA	LYS I	101	55.447	58.221	179.545	1.00 51.84	D
ATOM	5990	CB	LYS I	101	56.544	57,170	179.363	1.00 54.60	D
ATOM	5991	CG	LYS I		57.883		180.006	1.00 60.79	D
MOTA	5992	CD	LYS I		58.895		179.789	1.00 60.46	D
MOTA	5993	CE	LYS I	101	60.217	56.724	180.447	1.00 60.70	D
MOTA	5994	NZ	LYS I	101 •	61.105	55.546	180.307	1.00 60.74	D
ATOM	5995	C	LYS I	101	55.990	59.615	179.226	1.00 49.53	D
ATOM	5996	Ō	LYS I		55.843		178.103	1.00 43.87	D
		N	PRO I		56.603		180.215		
MOTA	5997							1.00 50.95	D
MOTA	5998	CD		102	56.554		181.666	1.00 51.41	D
MOTA	5999	CA	PRO I	102	57.138	61.633	179.952	1.00 48.65	, D
ATOM	6000	CB	PRO I	102	57.318	62.223	181.358	1.00 48.03	D
MOTA	6001	CG	PRO I	102	56.336	61.456	182.187	1.00 52.32	D
ATOM	6002	C	PRO I	102	58.456	61.574	179.202	1.00 42.44	D
ATOM	6003	ō	PRO I		59.088		179.111	1.00 42.74	Ď
									•
MOTA	6004	N	TRP I		58.842		178.631	1.00 37.59	D
MOTA	6005	CA	TRP I		60.113	62.806	177.935	1.00 37.08	D
ATOM	6006	CB	TRP I	103	59.891	63.519	176.604	1.00 30.32	D
ATOM	6007	CG	TRP I	103	61.104	63.612	175,767	1.00 30.53	D
ATOM	6008	CD2	TRP I	103	61.554	64.766	175.056	1.00 26.12	D
ATOM	6009	CE2	TRP I		62.738		174.378	1.00 19.41	D
MOTA	6010	CE3	TRP I		61.070		174.925	1.00 26.01	D
ATOM	6011		TRP I		62.007		175.503	1.00 27.90	D
MOTA	6012	NE1	TRP I	103	62.992	63.088	174.668	1.00 22.50	D
MOTA	6013	CZ2	TRP I	103	63.450	65.307	173.581	1.00 17.75	D
MOTA	6014	CZ3	TRP I	103	61.785	66.971	174.129	1.00 24.48	D
ATOM	6015 -	CH2	TRP I	103	62.959	66,578	173.470	1.00 16.99	D
ATOM	6016	C	TRP I				178.961	1.00 37.08	- D
ATOM	6017	.0	TRP I		60.713		179.043	1.00 35.25	D
			PRO I				179.784		
MOTA	6018	И			61.725			1.00 35.50	D
ATOM	6019	CD	PRO I		62.203		179.464	1.00 35.72	D
ATOM	6020	CA	PRO I		62.546		180.848	1.00 31.52	D
MOTA	6021	CB	PRO I		63.165		181.483	1.00 25.01	D
MOTA	6022	CG	PRO I	104	63.458	61.520	180.310	1.00 27.01	D
ATOM	6023	С	PRO I	104	63.585	64.588	180.369	1.00 30.56	. D
ATOM	6024	0	PRO I	104	64.766	64.267	180.236	1.00 32.35	· D
MOTA	6025	N	VAL I		63.124		180.111	1.00 27.61	D
								1.00 27.01	
MOTA	6026		VAL I		63.981		179.653		D
MOTA	6027	CB	VAL I		63.753		178.164	1.00 26.67	D
MOTA	6028		VAL I		64.776	68.243	177.714	1.00 23.05	D
MOTA	6029	CG2	VAL I	105	63.866		177.324	1.00 27.52	D
MOTA	6030	С	VAL I	105	63.630	68.097	180.457	1.00 29.50	D
ATOM	6031	0	VAL I		62.447		180.635	1.00 25.92	D
ATOM	6032	N	ALA I		64.662		180.958	1.00 33.08	D
MOTA	6033	CA	ALA I		64.467		181.718	1.00 35.06	D
MOTA	6034	CB.	ALA I		64.361		183.184	1.00 34.44	D
MOTA	6035	С	ALA I		65.632	70.926	181.450	1.00 37.67	D
MOTA	6036	0	ALA I	106	66.787	70.499	181.335	1.00 37.45	D
MOTA	6037	N	LEU I		65.296	72,202	181.319	1.00 40.17	D
ATOM	6038	CA	LEU I		66.262		181.074	1.00 41.87	D
ATOM	6039	CB	LEU I		65.682		180.100	1.00 38.48	D
							178.627		
ATOM	6040	CG	LEU I		66.105			1.00 38.10	D
MOTA	6041	CDI	LEU I) TO /	66.346	12.787	178.187	1.00 31.73	D

MOTA	6042	CD2	LEU D	107	65.047	74.879 177.78	1 1.00 30.60	D
MOTA	6043	C	LEU D	107	66.551	73.929 182.39	7 1.00 41.81	D
ATOM	6044	0	LEU D	107	65.630	74.287 183.13		D
MOTA	6045	N	TYR D		67.832	74.056 182.71		D
ATOM	6046	CA	TYR D		68.270	74.728 183.93		D
ATOM	6047	CB	TYR D		69.165	73.817 184.77		D
ATOM	6048	CG	TYR D		68.361	72.833 185.57		D
ATOM	6049	CD1			68.100	71.555 185.08		D
ATOM	6050	CE1			67.299	70.663 185.79		Ď
ATOM	6051	CD2	TYR D		67.804	73.200 186.79		D
ATOM	6052	ĊE2	TYR D		67.002	72.325 187.51		D
ATOM	6053	CZ	TYR D			71.054 187.01		D
ATOM	6054	ОН	TYR D	-	65.951	70.174 187.73		D
ATOM	6055	C	TYR D		69.018	75.966 183.47		Ď
ATOM	6056	ŏ	TYR D		70.147	75.886 182.99		D
ATOM	6057	N	LEU D		68.356	77.109 183.59		D
ATOM	6058	CA	LEU D		68.919	78.364 183.12		D
ATOM	6059	CB	TEA D		67.960	78.981 182.10		D
ATOM	6060	CG	LEU D		67.440	78.021 181.02		D
ATOM	6061		LEU D		66.449	78.741 180.11		D
ATOM	6062		LEU D		68.607	77.467 180.24		D
ATOM	6063	C	LEU D		69.220	79.391 184.20		D
ATOM	6064	ō	LEU D		68.346	79.718 185.00		D
ATOM	6065	И	THR D		70.455	79.901 184.21		D
MOTA	6066	CA	THR D		70.433	80.907 185.17		D
ATOM	6067	CB	THR D		72.131	80.447 185.95		D
ATOM	6068	OG1	THR D		71.867	79.178 186.55		
MOTA	6069	CG2						D
ATOM	6070	C	THR D		72.466 71.246	81.446 187.05 82.209 184.48		D
ATOM	6071	0	THR D		72.117	82.248 183.59		D
ATOM	6072	N	PRO D		70.578	83.302 184.87		D
MOTA	6072	CD	PRO D		69.529	83.398 185.89		D
ATOM	6074	CA	PRO D		70.826			D
ATOM	6075	CB	PRO D			84.613 184.26		D
ATOM	6076	CG	PRO D		69.827 68.750	85.529 184.98		D
ATOM	6077	C	PRO D			84.606 185.42		D
			PRO D		72.255 72.867	85.056 184.49		D
MOTA	6078	0				84.709 185.51		D
ATOM	6079	N	VAL D		72.782	85.814 183.54		D
ATOM	6080	CA CB	VAL D		74.138 74.788	86.330 183.64		D
ATOM ATOM	6081 6082		VAL D			86.531 182.26		D
	6083	CG2	VAL D		75.008	85.173 181.59		D
MOTA			VAL D		73.907	87.438 181.39		D
ATOM ATOM	6084 6085	0	VAL D		74.069 73.026	87.664 184.36	•	D
		N	SER D		75.176	88.320 184.36 88.058 184.98		D
ATOM	6086 6087	CA	SER D		75.222			D
MOTA	6088			-		89.323 185.70		D
MOTA		CB	SER D		76.641	89.599 186.19		D
MOTA	6089	OG	SER D		77.519	89.755 185.09		D
ATOM	6090	C	SER D		74.760	90.492 184.84		D
ATOM	6091	0	SER D		74.220	91.475 185.35		D
ATOM	6092	N	SER D		74.968	90.384 183.53		D
ATOM	6093	CA	SER D		74.584	91.454 182.63		D
MOTA	6094	CB	SER D		75.488	91.434 181.39		D
MOTA	6095	OG C	SER D		75.306	90.260 180.64		D
MOTA	6096	C	SER D		73.118	91.429 182.20		D
ATOM	6097	0	SER D		72.658	92.311 181.49		D
ATOM	6098	N .	ALA D		72.380	90.429 182.66		D
MOTA	6099	CA	ALA D	T12	70.972	90.306 182.32	3 1.00 55.17	D

MOTA	6100	CB	ALA D	115	70.392	89.074 182.	999 1.00	59.33	D
ATOM	6101	C	ALA D	115	70.163	91.548 182.	712 1.00	56.57	D
ATOM	6102	0	ALA D	115	.70.132	91.937 183.	886 1.00	53.06	D
ATOM	6103	N	GLY D		69.490	92.143 181.	720 1.00	58.70	D
ATOM	6104	CA	GLY D		68.687	93.339 181.		57.98	D
ATOM	6105	C	GLY D	-	67.607	93.244 183.		54.13	D
MOTA	6106	ŏ	GLY D		67.875	92.986 184.		53.49	D
			GLY D						
MOTA	6107	N			66.378	93.504 182.		51.13	D
ATOM	6108	CA	GLY D		65.247	93.419 183.		49.54	D
ATOM	6109	C	GLY D		64.444	92.257 182.		45.32	D
MOTA	6110	0	GLY D		64.316	91.219 183.		41.28	D
MOTA	6111	N	VAL D		63.926	92.442 181.		43.53	D
ATOM	6112	CA	VAL D		63.172	91.418 181.		39.62	D
MOTA	6113	CB	VAL D		62.195	92.048 180.0	049 1.00	36.60	D
ATOM	6114	CG1	VAL D	118	61.689	91.006 179.0	068 1.00	33.90	D
MOTA	6115	CG2	VAL D	118	61.049	92.667 180.	325 1.00	37.97	Œ
ATOM	6116	С	VAL D	118	64.158	90.581 180.2	225 1.00	36.77	D
ATOM	6117	0	VAL D	118	64.528	90.966 179.3	139 1.00	40.52	D
ATOM	6118	N	ALA D	119	64.585	89.443 180.		33.72	D
ATOM	6119	CA	ALA D		65.538	88.595 180.0		32.65	D
ATOM	6120	CB	ALA D		66.347	87.804 181.0		30.48	D
ATOM	6121	c	ALA D		64.896	87.641 179.0		35.66	D
ATOM	6122	ō ·	ALA D		65.601	87.014 178.2		34.93	D
ATOM	6123	N	ILE D		63.571	87.513 179.0		35.52	· D
ATOM	6124	CA	ILE D		62.824	86.658 178.3			
		CB	ILE D		62.596			34.90	D
ATOM	6125					85.264 178.7		38.09	D
MOTA	6126	CG2	ILE D		61.650	84.470 177.8		30.29	D
MOTA	6127	CG1	IFE D		63.921	84.527 178.9		38.37	D
ATOM	6128	CD1	ILE D		63.783	83.171 179.		36.87	D
MOTA	6129	C	ILE D		61.449	87.280 177.9		37.61	D
ATOM	6130	0	ITE D		60.647	87.462 178.8		41.13	D
MOTA	6131	N	LYS D	121	61.168	87.600 176.6	543 1.00	32.47	D
MOTA	6132	CA	LYS D	121	59.880	88.193 176.3	321 1.00	36.26	D
MOTA	6133	CB	LYS D	121	59.930	88.923 174.9	968 1.00	46.31	D
ATOM	6134	CG	LYS D	121	60.415	90.375 174.9	977 1.00	49.15	D
MOTA	6135	CD	LYS D	121	61.887	90.475 175.3		62.54	D
ATOM	6136	CE	LYS D	121	62.463	91.829 174.9	973 1.00	65.40	D
MOTA	6137	NZ	LYS D	121	62.286	92.089 173.5	509 1.00	67.14	D
ATOM	6138	C	LYS D		58.693	87.227 176.2		35.22	D
ATOM	6139	ō	LYS D		58.786	86.070 175.8		33.57	D
ATOM	6140	N	ALA D		57.564	87.732 176.		33.71	D
ATOM	6141	CA	ALA D		56.339	86.971 176.		33.24	. D
ATOM	6142	CB	ALA D		55.205	87.794 177.3		19.80	D D
ATOM	6143	CD	ALA D		56.042	86.691 175.2		34.23	D
	6144		ALA D		56.042				D
ATOM		0				87.606 174.4		35.03	
ATOM	6145	N	GLY D		55.783	85.428 174.9		32.35	D
ATOM	6146	CA	GLY D		55.464	85.053 173.		31.57	D
MOTA	6147	C	GLY D		56.649	84.707 172.6		31.64	D
MOTA	6148	0	GLY D		56.478	84.377 171.		33.03	D
ATOM	6149	N	SER D		57.854	84.750 173.2		30.96	D
MOTA	6150	CA	SER D		59.031	84.474 172.4		31.06	D
MOTA	6151	CB	SER D		60.210	85.334 172.		31.98	D
MOTA	6152	OG	SER D	124	60.508	85.135 174.2		21.85	D
MOTA	6153	C	SER D	124	59.479	83.019 172.2	296 1.00	32.52	D
MOTA	6154	0	SER D	124	59.207	82.169 173.	147 1.00	31.79	D
ATOM	6155	N	LEU D		60.187	82.740 171.2		31.44	D
ATOM	6156	CA	LEU D		60.692	81.402 171.0		31.36	D
ATOM	6157	CB	LEU D		61.200	81.196 169.		29.94	D

ATOM	6158	CG	LEU D	125	61.949	79.870	169.410	1.00 28.	69 D
MOTA	6159	CD1	LEU D	125	60.979	78.717	169.659	1.00 15.	
MOTA	6160		LEU D		62.569	79.778	168.036	1.00 22.	
MOTA	6161	С	TEA D		61.841		171.957	1.00 28.	
ATOM	6162	0	LEU D	125	62.789		171.833	1.00 31.	
MOTA	6163	N	ILE D		61.749		172.914	1.00 32.	
ATOM	6164	CA	ILE D		62.771		173.933	1.00 33.0	
MOTA	6165	CB	ILE D		62.081		175.298	1.00 35.	
ATOM	6166	CG2	ILE D		62.463		175.962	1.00 23.0	
MOTA	6167	CG1	ILE D		62.341		176.127	1.00 30.0	
ATOM	6168	CD1	ILE D		61.580		177.402	1.00 53.9	
ATOM	6169	C	ILE D		63.726		173.634	1.00 33.0	_
ATOM	6170	ō	ILE D		64.889		173.968	1.00 31.4	
ATOM	6171	N	ALA D		63.237		172.989	1.00 32.	
ATOM	6172	CA	ALA D		64.079		172.657	1.00 29.0	_
ATOM	6173	CB	ALA D		64.422		173.918	1.00 25.	
ATOM	6174	C	ALA D		63.450		171.652	1.00 27.	
ATOM	6175	ō ·	ALA D		62.229		171.498	1.00 30.6	
ATOM	6176	N	VAL D		64.298		170.959	1.00 20.0	
ATOM	6177	CA	VAL D		63.828		170.021	1.00 21.9	
ATOM	6178	CB	VAL D		64.206		168.564	1.00 21.5	
ATOM	6179		VAL D		63.886		167.659	1.00 21.0	
ATOM	6180	CG2			63.418		168.086	1.00 20.2	_
MOTA	6181	C	VAL D		64.505		170.421	1.00 26.3	
ATOM	6182	Õ	VAL D		65.734		170.435	1.00 28.6	
ATOM	6183	N	LEU D		63.710		170.433	1.00 24.5	_
ATOM	6184	CA	LEU D		64.254		171.169	1.00 24.5	
ATOM	6185	CB	LEU D		63.726		172.548	1.00 26.5	-
MOTA	6186	CG	PEA D		64.049		173.685	1.00 28.5	
MOTA	6187	CD1			63.480		174.970	1.00 18.7	
MOTA	6188		LEU D		65.565		173.813	1.00 34.0	
ATOM	6189	C	PEA D		63.910		170.183	1.00 34.0	
MOTA	6190	Ö	PEA D		62.734		169.860		
ATOM	6191	N	ILE D		64.940		169.714	1.00 31.2	
MOTA	6192	CA	ILE D		64.725		168.761	1.00 28.1	
ATOM	6193	CB	ILE D		65.699		167.566	1.00 29.8	
ATOM	6194	CG2			65.502		166.632	1.00 29.6	
ATOM	6195	CG1	ILE D		65.424		166.779	1.00 24.6	·-
ATOM			ILE D		66.417		165.682	1.00 26.5	
ATOM	6197	C	ILE D		64.842		169.382	1.00 35.5	
ATOM	6198	Ö	ILE D		65.910		169.858	1.00 31.0	
ATOM	6199	N	LEU D		63.710		169.356	1.00 30.2	
ATOM	6200	CA	LEU D		63.575		169.876	1.00 33.2	
ATOM	6201	CB	LEU D		62.174		170.454	1.00 31.2	
ATOM	6202	CG	LEU D		61.878		171.089	1.00 25.4	
ATOM	6203	-	LEU D		60.662		171.009	1.00 34.2	
ATOM	6204		LEU D		. 61.670		170.002	1.00 34.2	
MOTA	6205	C	LEU D		63.787		168.702	1.00 30.9	
ATOM	6206	õ	LEU D		63.101		167.699		•
ATOM	6207	N	ARG D		64.743		168.833	1.00 30.9 1.00 34.5	
ATOM	6208	CA	ARG D		65.042		167.778	1.00 34.5	
MOTA	6209	CB	ARG D						
ATOM	6210		ARG D		66.511 66.934		167.409	1.00 31.7	
MOTA	6211	CG	ARG D				166.377	1.00 25.0	
	6212	CD			68.340		166.004	1.00 30.9	
ATOM	6213	NE	ARG D		68.698		164.702	1.00 48.1	
ATOM ATOM	6214	CZ	ARG D		69.821		164.059	1.00 54.0	
MOTA					70.689		164.605	1.00 54.7	
ATOM	6215	MUZ	ARG D	T27	70.078	60.T/3	162.866	1.00 55.9	6 D

MOTA	6216	С	ARG :	D	132	64.700	60.139	168.244	1.00	38.33	D
MOTA	6217	0	ARG :	D	132	65.256	59.648	169.230	1.00	38.52	D
ATOM	6218	N	GLN :	D	133	63.792	59.494	167.513	1.00	38.39	D
MOTA	6219	CA	GLN :	D	133	63.317	58.158	167.850	1.00	33.51	D
MOTA	6220	CB	GLN :	D	133	61.819	58.212	168.123	1.00	30.61	D
MOTA	6221	CG	GLN :	D	133	61.149	56.859	168.321	1.00	39.48	D
MOTA	6222	CD	GLN :	D	133	60.552	56.280	167.045	1.00	36.71	D
ATOM	6223	OE1	GLN :	D	133	59.736	56.910	166.382	1.00	41.51	D
MOTA	6224	NE2	GLN :	D	133	60.955	55.069	166.708	1.00	35.25	D
MOTA	6225	C	GLN :	D	133	63.600	57.110	166.796	1.00	34.18	D
MOTA	6226	0	GLN :	D	133	63.279	57.281	165.620	1.00	36.28	D
ATOM	6227	N	THR :	D	134	64.215	56.023	167.241	1.00	33.02	D
MOTA	6228	CA	THR :	D	134	64.547	54.876	166.398	1.00	32.17	D
MOTA	6229	CB	THR :	D	134	66.044	54.702	166.287	1.00	30.15	D
MOTA	6230	OG1	THR :	D	134	66.609	54.883	167.593	1.00	44.11	D
MOTA	6231	CG2	THR :	D	134	66.634	55.692	165.317	1.00	22.68	D
MOTA	6232	C	THR :	D	134	63.982	53.630	167.101	1.00	35.50	D
MOTA	6233	0	THR :			63.174	.53.739	168.037	1.00	32.36	D
ATOM	6234	N	ASN :	D	135	64.404	52.445	166.669	1.00	35.58	D
MOTA	6235	CA	ASN :	D	135	63.902	51.237	167.304	1.00	41.05	D
ATOM	6236	CB	ASN :	D	135	62.469	50.964	166.859	1.00	40.87	D
MOTA	6237	CG	ASN I			62.345	50.879	165.360	1.00	41.94	D
MOTA	6238	OD1				63.211	50.322	164.689	1.00	43.65	D.
MOTA	6239	ND2	ASN :	D	135	61.266	51.429	164.823	1.00	41.79	D
MOTA	6240	С	ASN 1			64.754	50.029	166.993	1.00	43.39	D
MOTA	6241	0	ASN 1			65.665	50.093	166.163		43.85	D
ATOM	6242	N	ASN I	D	136	64.449	48.927	167.669	1.00	44.82	D
MOTA	6243	CA	ASN :	D	136	65.166	47.679	167.450	1.00	49.97	· D
MOTA	6244	CB	ASN :			65.318	46.917	168.753	1.00	49.65	D
MOTA	6245	CG	ASN :			63.987	46.597	169.388	1.00	55.20	D
MOTA	6246	OD1	ASN I			63.924	46.031	170.481	1.00	58.92	Ð
MOTA	6247	ND2				62.907		168.709	1.00	55.27	· D
ATOM	6248	C	ASN :			64.371		166.481		53.16	D
MOTA	6249	0	ASN :			64.345		166.601	1.00	53.71	D
ATOM	6250	N	TYR :			63.704		165.534	1.00	55.41	D
ATOM	6251	CA	TYR :			62.903		164.566	1.00	55.16	D
MOTA	6252	CB	TYR :			61.416		164.769		60.51	D
ATOM	6253	CG	TYR :			60.548		163.824		71.04	D
ATOM	6254	CD1						163.763	1.00	68.96	Ď
ATOM	6255		TYR			59.861		162.880		72.76	D
ATOM	6256	CD2	TYR :			59.637		162.972	1.00	75.48	D
ATOM	6257	CE2	TYR :			58.845		162.084	1.00	74.32	D
ATOM	6258	CZ	TYR			58.964		162.046	1.00	73.15	D
MOTA	6259	OH	TYR			58.184		161.179	1.00	72.59	D
ATOM	6260	C	TYR			63.266		163.123		52.42	D
MOTA	6261	0	TYR			63.283		162.329		54.24	. D
ATOM	6262	N	ASN			63.553		162.776		49.30	D
ATOM	6263	CA	ASN ASN			63.916		161.399 160.540		49.09	D
ATOM	6264	CB				62.667		-		48.86	D
MOTA MOTA	6265	CG			138	61.705		161.051 160.517		44.77	D
	6266		ASN			60.623				46.88	. D
MOTA MOTA	6267 6269		ASN			62.095		162.084 161.279		44.57	D
ATOM	6268	C	ASN			64.727				52.13	D
ATOM	6269	O	ASN			65.282 64.790		162.268		54.23	D
ATOM	6270 6271	N	SER					160.071		52.55	D
ATOM	6271 6272	CA CB	SER SER			65.564 66.094		159.857 158.418		52.05	D
MOTA	6273	OG	SER			65.031		158.418		54.53 64.83	D
277 014	02/3	00	JER	•	100	33.031	31.133	-J1.40U	Ŧ.00	94.93	D

MOTA	6274	С	SER D	139	64.828	52.974 160.170	1.00 45.51	D
MOTA	6275	0	SER D	139 .	65.229	54.038 159.699	1.00 41.72	D.
MOTA	6276	N	ASP D	140	63.763	52.895 160.965	1.00 43.15	D
ATOM	6277	CA	ASP D	140	63.003	54.086 161.340	1.00 44.07	D
MOTA	6278	CB	ASP D	140	61.744	53.694 162.129	1.00 42.00	D
MOTA	6279	CG	ASP D	140	60.593	53.266 161.228	1.00 44.72	D
MOTA	6280	OD1	ASP D	140	59.534	52.848 161.755	1.00 39.06	D
MOTA	6281	OD2	ASP D	140	60.743	53.350 159.987	1.00 44.25	D
MOTA	6282	C	ASP D	140	63.843	55.077 162.163	1.00 44.58	D
MOTA	6283	0	ASP D	140	64.341	54.757 163.241	1.00 40.77	D
MOTA	6284	N	ASP D	141	63.990	56.286 161.639	1.00 46.87	D
MOTA	6285	CA	ASP D	141	64.747	57.345 162.302	1.00 44.40	D
ATOM	6286	CB	ASP D	141	66.113	57.487 161.636	1.00 48.13	D
MOTA	6287	CG	ASP D	141	67.092	58.291 162.464	1.00 54.26	D
MOTA	6288	OD1	ASP D	141	66.660	59.093 163.322	1.00 56.40	D
MOTA	6289	OD2	ASP D	141	68.307	58.126 162.235	1.00 58.45	D
MOTA	6290	С	ASP D	141	63.930	58.628 162.103	1.00 41.56	D
MOTA	6291	0	ASP D		64.118	59.342 161.116	1.00 42.25	· D
MOTA	6292	N	PHE D		63.022	58.906 163.031	1.00 34.64	D
MOTA	6293	CA	PHE D		62.154	60.074 162.930	1.00 35.62	D
ATOM	6294	CB	PHE D		60.691	59.659 163.148	1.00 32.21	D
MOTA	6295	CG	PHE D		60.208	58.613 162.189	1.00 36.37	D
ATOM	6296		PHE D		59.562	57.468 162.659	1.00 40.98	D
MOTA	6297		PHE D		60.361	58.777 160.812	1.00 28.49	D
MOTA	6298		PHE D		59.065	56.503 161.769	1.00 34.40	D
ATOM	6299		PHE D		59.873	57.829 159.927	1.00 30.18	D
MOTA	6300	CZ	PHE D		59.221	56.688 160.408	1.00 32.89	D
ATOM	6301	C	PHE D		62.508	61.172 163.921	1.00 37.65	D
MOTA	6302	0	PHE D		63.052		1.00 39.93	D
ATOM	6303	N	GLN D		62.178	62.405 163.559	1.00 35.40	D
ATOM	6304	CA	GLN D		62.467	63.531 164.426	1.00 30.59	D
ATOM	6305	CB	GLN D		63.374	64.531 163.726	1.00 26.22	D
ATOM	6306	CG	GIM D		64.757	64.051 163.426	1.00 31.74	D
ATOM	6307	CD	GLN D		65.664	65.204 163.100	1.00 44.27	D
ATOM	6308		GLN D		65.267	66.123 162.384	1.00 45.79	D
ATOM	6309	NE2			66.892	65.176 163.626	1.00 52.76	D
ATOM	6310	C	GLN D		61.204	64.244 164.848	1.00 30.08	D
ATOM	6311	0	GLN D		60.353	64.562 164.025	1.00 30.98	D
MOTA	6312	N	PHE D		61.093	64.484 166.145	1.00 30.40	D
ATOM	6313	CA	PHE D		59.953	65.176 166.706	1.00 28.23	D D
ATOM	6314	CB ·	PHE D		59.343	64.366 167.841 63.113 167.379	1.00 27.48 1.00 27.17	D
MOTA	6315	CG	PHE D		58.663 59.398	62.061 166.845	1.00 27.17	. D
MOTA ATOM	6316 6317		PHE D		57.278	62.981 167.476	1.00 27.01	D
ATOM	6318		PHE D		58.759	60.885 166.414	1.00 23.50	D
ATOM	6319		PHE D		56.633		1.00 23.30	D
ATOM	6320	CEZ	PHE D		57.379	60.768 166.521	1.00 19.26	Ď
ATOM	6321	C	PHE D		60.495		1.00 28.85	ā
ATOM	6322	ō	PHE D		61.233	66.516 168.194	1.00 31.92	D
ATOM	6323	N	VAL D		60.123	67.570 166.527	1.00 23.53	D
ATOM	6324	CA	VAL D		60.608	68.880 166.878	1.00 21.18	D
ATOM	6325	CB	VAL D		60.867	69.693 165.609	1.00 23.24	D
ATOM	6326		VAL D			71.061 165.972	1.00 18.08	ā
ATOM	6327		VAL D		61.889	68.965 164.719	1.00 18.41	ā
ATOM	6328	C	VAL D		59.692	69.649 167.789	1.00 26.00	D
ATOM	6329	Õ	VAL D		58.523	69.850 167.475	1.00 33.86	ā
ATOM	6330	N	TRP D		60.222	70.085 168.928	1.00 27.40	D
ATOM	6331	CA	TRP D		59.424	70.853 169.882	1.00 26.75	D
					· -		· -	-

MOTA	6332	CB	TRP D	146	59.506	70.212	171.275	1.00	25.43	D
MOTA	6333	·CG	TRP D	146	59.261	68.728	171.236	1.00	27.11	, D
MOTA	6334	CD2	TRP D	146	57.992	68.065	171.210	1.00	23.03	D
MOTA	6335	CE2	TRP D	146	58.246	66.681	171.078	1.00	26.00	D
MOTA	6336	CE3	TRP D	146	56.663	68.505	171.278	1.00	24.17	D
MOTA	6337	CD1	TRP D	146	60.205	67.747	171.124	1.00	27.33	D
ATOM	6338	NE1	TRP D	146	59.605	66.515	171.025	1.00	30.19	D
ATOM	6339	CZ2	TRP D	146	57.217	65.730	171.022		24.41	D
ATOM	6340	CZ3	TRP D	146	55.629	67.547	171.217	1.00	22.87	D
MOTA	6341	CH2	TRP D	146	55.919		171.092		16.39	D
ATOM	6342	C	TRP D		59.878		169.925		28.37	D
MOTA	6343	0	TRP D		61.049		170.175		28.62	D
ATOM	6344	N	ASN D	-	58.951		169.642		27.25	D
MOTA	6345	CA	ASN D		59.271		169.667		26.16	D
ATOM	6346	CB	ASN D		58.650		168.456		23.89	D
ATOM	6347	CG	ASN D		59.114		167.134		27.09	D
ATOM	6348		ASN D		60.314		166.898		20.08	D
ATOM	6349		ASN D		58.167		166.263		29.99	D
ATOM	6350	C	ASN D		58.729		170.969		26.56	D
ATOM	6351	Ō	ASN D		57.512		171.140		27.81	ם מ
ATOM	6352	N	ILE D		59.639		171.884		24.13	D
ATOM	6353	CA	ILE D		59.260		173.197		25.61	D
ATOM	6354	СВ	ILE D		60.325		174.261		27.27	Ď
ATOM	6355	CG2	ILE D		59.691		175.646		27.75	Ď
MOTA	6356	CG1	ILE D		60.980		173.935		29.39	D
ATOM	6357	CD1			60.068		173.920		17.68	D
ATOM	6358	C	ILE D		59.072		173.264		24.39	D
ATOM	6359	ō	ILE D		60.029		173.129		31.25	D
ATOM	6360	N.	TYR D		57.849		173.479		21.31	· D
ATOM	6361	CA	TYR D		57.577		173.608		26.14	D
MOTA	6362	CB	TYR D		56.372		172.753		22.48	D
ATOM	6363	CG	TYR D		56.648		171.275		26.88	D
ATOM	6364		TYR D		56.710		170.523		28.49	D
ATOM	6365	CE1	TYR D		56.985		169.166		27.20	D
ATOM	6366	CD2	TYR D		56.870		170.623		30.75	D
ATOM	6367	CE2	TYR D		57.150		169.261		29.69	D
ATOM	6368	CZ	TYR D		57.204		168.538		31.37	ā
ATOM	6369	OH	TYR D		57.469		167.190		32.39	Ď
ATOM	6370	C	TYR D		57.279		175.076		30.05	D
ATOM	6371	Ö	TYR D		56.691		175.800		34.32	D
ATOM	6372	N	ALA D		57.687		175.514		31.39	ā
ATOM	6373	CA	ALA D		57.420	-	176.880		30.53	D
ATOM	6374	CB	ALA D		58.557		177.398		25.01	D
ATOM	6375	C	ALA D		56.160		176.847		32.63	D
ATOM.	6376	ō	ALA D		56.033		176.011		37.10	Ď
ATOM	6377	N	ASN D		55.230		177.755			D
ATOM	6378	CA	ASN D		53.975		177.773		31.76	D
ATOM	6379	CB	ASN D		52.896		178.500		37.84	ā
ATOM	6380	CG	ASN D		52.346		177.671		41.40	D
ATOM	6381		ASN D		51.861		176.557		42.29	D
ATOM	6382		ASN D		52.413				39.30	
ATOM	6383	C	ASN D				178.213 178.446			D
ATOM			ASN D		54.076				32.29	D
	6384	O N	ASN D		53.235		178.238		36.96	D
ATOM	6385	N			55.111		179.253		31.47	D
ATOM	6386	CA	ASN D		55.271		180.014		30.73	D
ATOM	6387	CB	ASN D		54.772		181.421		29.45	D
MOTA	6388	CG	ASN D		55.627		182.155		33.46	D
MOTA	6389	ODI	ASN D	152	55.540	82.991	181.906	1.00	42.29	D

MOTA	6390	ND2	ASN D	152	56.478	84.679 183	3.050	1.00	34.86	D
MOTA	6391	C	ASN D		56.710	85.944 186	0.102	1.00	32.32	D
MOTA	6392	0	ASN D	152	57.652	85.201 179	9.777	1.00	22.60	D
MOTA	6393	N	ASP D	153	56.868	87.185 180	0.576	1.00	32.96	D
MOTA	6394	CA	ASP D	153	58.199	87.758 180		1.00	34.17	D
MOTA	6395	CB	ASP D	153	58.175	89.275 180	0.989	1.00	33.81	D
ATOM	6396	CG	ASP D		57.575	90.087 179	9.852	1.00	41.74	D
MOTA	6397		ASP D		57.581	89.650 178	8.674	1.00	43.26	D
MOTA	6398	OD2	ASP D	153	57.116	91.206 180	0.162	1.00	36.22	D
ATOM	6399	C	ASP D	153	58.869	87.150 183	1.951	1.00	33.17	D
ATOM	6400	0	ASP D	153	58.223	86.915 182	2.966	1.00	33.49	D
MOTA	6401	N	VAL D	154	60.162	86.891 183	1.833	1.00	30.92	D
MOTA	6402	CA	VAL D	154	60.959	86.421 182	2.943	1.00	31.38	D
MOTA	6403	CB	VAL D	154	61.767	85.188 182	2.585	1.00	33.39	a
MOTA	6404		VAL D		62.727	84.833 183		1.00	29.51	D
ATOM	6405	CG2	VAL D		60.843	84.060 182	2.308	1.00	37.67	D
MOTA	6406	C	VAL D	154	61.939	87.572 183		1.00	33.41	D
MOTA	6407	0	VAL D		62.927	87.798 182		1.00	30.75	D
ATOM	6408	N	VAL D	155	61.639	88.309 184	1.321	1.00	34.81	D
ATOM	6409	CA	VAL D		62.469	89.429 184	1.754	1.00	34.30	D
MOTA	6410	CB	VAL D		61.635	90.516 185		1.00	33.55	D
ATOM	6411		VAL D		62.560	91.436 186	5.289	1.00	37.26	D
MOTA	6412	CG2			60.807	91.337 184			38.10	D
MOTA	6413	C	VAL D		63.586	88.996 185		1.00	32.23	D
MOTA	6414	0	VAL D		63.384	88.172 186	5.581	1.00	29.51	D
ATOM	6415	N	VAL D		64.766	89.563 185			35.10	D
ATOM	6416	CA	VAL D		65.929	89.321 186		1.00	38.71	,. D
ATOM	6417	CB	VAL D		67.150	88.920 185		1.00	42.06	D
MOTA	6418		VAL D		68.394	89.027 186			36.41	D
ATOM	6419		VAL D		66.962	87.497 184		1.00	41.89	D
ATOM	6420	C	VAL D		66.220	90.665 186		1.00	38.78	D
ATOM	6421	0	VAL D		66.744	91.570 186			41.23	D
ATOM	6422	N	PRO D		65.890	90.813 188			38.55	D
ATOM	6423	CD	PRO D		65.442	89.754 189			37.36	D
MOTA	6424	CA	PRO D		66.109	92.064 189			38.18	D
ATOM	6425	CB	PRO D		65.747	91.689 190			37.79	D
ATOM	6426	CG	PRO D		64.770	90.555 190			38.73	D
ATOM	6427	G	PRO D		67.527	92.605 188			36.55	D
ATOM	6428	0	PRO D		68.503	91.836 188			36.02	· D
MOTA	6429	N	THR D		67.638	93.928 188			32.19	D
ATOM	6430	CA	THR D		68.953	94.542 188			37.42	D
ATOM	6431	CB	THR D		68.867	95.995 188			41.41	D
MOTA	6432	OG1	THR D		70.150	96.610 188			46.90	D
ATOM	6433	CG2	THR D		67.862	96.741 189			46.90	D
ATOM ATOM	6434	C	THR D	· ·	69.621	94.484 190			36.73	D
	6435	0	THR D		68.974	94.742 191			34.96	ď
MOTA	6436	N	GLY D		70.906	94.124 190			35.62	D
ATOM	6437 6438	CA	GLY D		71.643	94.028 191			36.28	D
ATOM		C	GLY D		72.313	95.316 191			37.83	. D
ATOM	6439 6440	0	GLY D		72.196	96.379 191			35.38	D
ATOM	6441	N			73.000	95.237 193			35.09	D
ATOM		CA	GLY D		73.672	96.418 193			36.59	D
ATOM	6442	C			75.037	96.477 192			37.35	D
MOTA MOTA	6443 6444	O NT	GLY D		75.482 75.709	95.471 192 97.625 192			38.20 37.82	D
	6445	N	CYS D		77.035	97.746 192				D
ATOM ATOM	6446	CA C	CYS D		78.174	97.290 193			40.12	D
ATOM	6447	0	CYS D		77.955	96.998 194			44.24	D D
WION	0441	J	CIO D	TOT	11.333	70.990 IJ	z . z 0 0	4.00	74.24	IJ

MOTA	6448	CB	CYS D	161	77.249	99.177	191.933	1.00 41.37	D
MOTA	6449	SG	CYS D	161	75.851	99.818	190.963	1.00 45.93	. D
ATOM	6450	N	ASP D	162	79.386	97.187	192.751	1.00 42.14	D
ATOM	6451	CA	ASP D	162	80.504	96.765	193.581	1.00 46.77	D
ATOM	6452	CB	ASP D	162	81.269	95.599	192.961	1.00 51.85	D
ATOM	6453	ÇG	ASP D	162	82.246	94.956	193.949	1.00 64.21	D
ATOM	6454	OD1	ASP D	162	81.835	94.651	195.095	1.00 64.19	D
ATOM	6455	OD2	ASP D	162	83.425	94.750	193.584	1.00 70.74	D
ATOM	6456	C	ASP D	162	81.438	97.930	193.801	1.00 50.77	D
MOTA	6457	0	ASP D	162	81.841	98.618	192.860	1.00 52.21	ם
ATOM	6458	N	VAL D	163	81.765	98.157	195.063	1.00 51.82	D
ATOM	6459	CA	VAL D		82.627	99.253	195.430	1.00 56.60	D
ATOM	6460	CB	VAL D		82.082		196.671	1.00 54.71	D
ATOM	6461	CG1	VAL D	163	83.012	101.072	197.094	1.00 56.74	D
ATOM	6462		VAL D			100.512		1.00 51.81	D
ATOM	6463	C	VAL D		84.030		195.666	1.00 64.32	D
ATOM	6464	0	VAL D		84.436		196.787	1.00 65.70	D
ATOM	6465	N	SER D		84.763		194.569	1.00 74.12	D
ATOM	6466	CA	SER D		86.134		194.573	1.00 81.28	ם
ATOM		CB	SER D		86.643		193.128	1.00 83.04	D
ATOM	6468	OG	SER D		85.623		192.250	1.00 74.81	D
ATOM	6469	C	SER D		87.020		195.383	1.00 86.27	D
ATOM	6470	ō	SER D			100.232		1.00 86.58	Ď
ATOM	6471	N	ALA D		87.475		196.541	1.00 90.59	D
ATOM	6472	CA	ALA D		88.348		197.426	1.00 95.36	D
ATOM	6473	CB	ALA D		87.565		198.648	1.00 94.09	D
ATOM	6474		ALA D		89.539		197.864	1.00 98.36	Ď
ATOM	6475	ŏ	ALA D		89.364		198.267	1.00101.61	Ď
ATOM	6476	N	ARG D		90.746		197.784	1.00 98.81	D
ATOM	6477	CA	ARG D		91.944		198.170	1.00 99.39	D
ATOM	6478	CB	ARG D		93.181		197.894	1.00 97.36	D
ATOM	6479	CG	ARG D		93.276		196.426	1.00 95.00	D
ATOM	6480	CD	ARG D			100.351		1.00 96.49	Ď
ATOM	6481	NE	ARG D			100.744		1.00 96.19	D
ATOM	6482	CZ	ARG D			101.551		1.00 94.46	. D
ATOM	6483		ARG D			102.062		1.00 91.13	D
ATOM	6484		ARG D			101.857		1.00 93.77	D
ATOM	6485	C	ARG D		91.888		199.629	1.00101.99	D
ATOM	6486	õ	ARG D		91.831		199.869	1.00104.31	D
ATOM	6487	N	ASP D		91.902		200.589	1.00101.69	D
ATOM	6488	CA	ASP D		91.805		202.027	1.00101.34	Ď
ATOM	6489	CB	ASP D		92.798		202.426	1.00104.24	Ď
ATOM	6490	CG	ASP D		92.590		203.868	1.00107.74	D
ATOM	6491		ASP D		93.471		204.390	1.00111.70	Ď
ATOM	6492		ASP D		91.547		204.483	1.00105.67	D
ATOM	6493	C	ASP D		92.012		202.967	1.00.09.65	. D
ATOM	6494	ō	ASP D			100.818		1.00101.50	. D
ATOM	6495	N	VAL D		92.461		204.187	1.00.95.26	מ
ATOM	6496	CA	VAL D			100.345		1.00 90.63	Ď
ATOM	6497	CB	VAL D		93.031		206.578	1.00 90.94	D
ATOM	6498		VAL D		94.050		206.354	1.00 90.94	ם
ATOM	6499		VAL D			100.620		1.00 92.62	ם
ATOM	6500	CGZ	VAL D			100.620		1.00 84.92	
			VAL D			101.250		1.00 84.92	D
ATOM ATOM	6501	O N	THR D			100.961		1.00 84.46	D
ATOM	6502	N CA	THR D			102.351		1.00 78.70	D
	6503		THR D			103.313			. D
MOTA	6504	CB	THR D					1.00 75.27	D
ATOM	6505	OGT	מ אחנ	707	J3.44U	103.984	ZUI./28	1.00 77.62	D

MOTA	6506	CG2	THR D	169	94.899	105.595	202.728	1.00 71.03	D
MOTA	6507	С	THR D	169	95.413	103.913	204.852	1.00 76.86	D
MOTA	6508	0	THR D	169	94.885	104.437	205.835	1.00 76.49	D
MOTA	6509	N	VAL D	170	96.727	103.836	204.671	1.00 77.26	D
MOTA	6510	CA	VAL D	170	97.668	104.391	205.629	1.00 78.22	D
MOTA	6511	CB	VAL D	170	99.063	103.713	205.533	1.00 81.59	D
MOTA	6512	CG1	VAL D	170	99.963	104.234	206.636	1.00 82.13	D
MOTA	6513	CG2	VAL D	170	98.931	102.196	205.647	1.00 84.36	D
ATOM	6514	C	VAL D	170	97.815	105.878	205.317	1.00 76.11	D
MOTA	6515	0	VAL D	170	98.574	106.270	204.431	1.00 68.50	D
MOTA	6516	N	THR D	171	97.049	106.692	206.038	1.00 79.42	D
ATOM	6517	CA	THR D	171	97.074	108.138	205.883	1.00 81.52	D
MOTA	6518	CB	THR D	171	95.830	108.799	206.575	1.00 77.65	D
MOTA	6519	OG1	THR D	171	95.976	110.219	206.591	1.00 81.79	Ď
ATOM	6520	CG2	THR D	171	95.686	108.336	207.997	1.00 73.42	D
ATOM	6521	C	THR D	171	98.362	108.598	206.552	1.00 85.52	D
MOTA	6522	0	THR D	171	98.392	109.612	207.251	1.00 88.94	D
ATOM	6523	N	LEU D	172	99.433	107.845	206.318	1.00 86.85	D
ATOM	6524	CA	LEU D	172	100.723	108.145	206.921	1.00 89.95	D
MOTA	6525	CB	LEU D	172	101.691	106.962	206.721	1.00 94.36	D
ATOM	6526	CG	LEU D	172	102.885	106.770	207.681	1.00 98.13	D
MOTA	6527	CD1	LEU D	172	103.458	105.362	207.512	1.00 98.63	D
MOTA	6528	CD2	TEA D	172	103.965	107.817	207.419	1.00 99.17	D
ATOM	6529	C	LEU D	172	101.393	109.450	206.480	1.00 89.07	D
ATOM	6530	0	TEA D	172	102.139	110.029	207.264	1.00 89.82	D
ATOM	6531	N	PRO D	173	101.137	109.939	205.244	1.00 86.42	D
ATOM	6532	CD	PRO D	173	100.015	109.681	204.328	1.00 84.78	D
ATOM	. 6533	CA	PRO D	173	101.807	111.193	204.872	1.00 85.56	. D
ATOM	6534	CB	PRO D	173			203.688	1.00 81.87	D
ATOM	6535	CG	PRO D	173	99.640	111.078	203.916	1.00 84.27	D
ATOM	6536.	C	PRO D	173	101.804	112.152	206.056	1.00 86.51	D
MOTA	6537	0	PRO D	173	100 :877	112.944	206.221	1.00 90.21	, D
ATOM	6538	N	ASP D	174		112.054		1.00 83.37	D
MOTA	6539	CA	ASP D	174	103.002	112.837	208.091	1.00 81.03	D
MOTA	6540	CB	ASP D	174	104.484	113.065	208.368	1.00 86.52	D
MOTA	6541	CG	ASP D			111.761		1.00 89.39	D
ATOM	6542		ASP D			110.999		1.00 90.18	D.
MOTA	6543		ASP D			111.487		1.00 96.23	D
MOTA	6544	C	ASP D			114.131		1.00 76.73	D
ATOM	6545	0	ASP D			114.861		1.00 72.49	D
ATOM	6546	N	TYR D			114.389		1.00 73.53	D
ATOM	6547	ÇA	TYR D			115.533		1.00 74.11	D
ATOM	6548	CB	TYR D			116.427		1.00 72.91	D
ATOM	6549	CG	TYR D			117.724		1.00 70.37	D
MOTA	6550		TYR D			117.718		1.00 67.23	D
ATOM	6551		TYR D			118.883		1.00 66.75	D
MOTA	6552		TYR D			118.939		1.00 69.48	Ø
MOTA	6553		TYR D			120.111		1.00 69.31	D
ATOM	6554	CZ	TYR D			120.071		1.00 64.14	D
ATOM	6555	OH	TYR D			121.220		1.00 65.72	D
MOTA	6556	C	TYR D			116.445		1.00 74.39	, D
MOTA	6557	0	TYR D			116.676		1.00 81.52	D
MOTA	6558	N	PRO D			117.015		1.00 66.94	D
MOTA	6559	CD	PRO D			117.251		1.00 59.18	D
MOTA	6560	CA	PRO D			117.868		1.00 61.40	D
MOTA	6561	CB	PRO D			118.838		1.00 60.17	D
ATOM	6562	CG	PRO D			117.956		1.00 64.68	D
MOTA	6563	С	PRO D	7.16	100.362	117.135	205.315	1.00 55.87	D

MOTA	6564	0	PRO D	176	99.509	117.627	204.572	1.00 50.21	D
MOTA	6565	N	GLY D	177	100.935	115.956	205.092	1.00 54.90	D
MOTA	6566	CA	GLY D	177			203.902	1.00 55.03	D
ATOM	6567	C.	GLY D	177	99.226	114.747	203.575	1.00 55.03	D
MOTA	6568	0	GLY D	177	98.361	114.693	204.448	1.00 59.29	D
ATOM	6569	N	SER D	178	98.998	114.431	202.301	1.00 49.88	D
MOTA	6570	CA	SER D	178	97.689	114.012	201.829	1.00 47.78	D
ATOM	6571	CB	SER D	178	96.922	115.213	201.269	1.00 43.67	D
MOTA	6572	OG	SER D	178			199.917	1.00 38.38	D
ATOM	6573	С	SER D	178			200.736	1.00 49.80	D
ATOM	6574	Ō	SER D	178			199.824	1.00 52.11	D
MOTA	6575	N	VAL D	179			200.820	1.00 51.59	· D
ATOM	6576	CA	VAL D	179	97.153	110.833	199.806	1.00 52.35	D
MOTA	6577	CB	VAL D	179			200.402	1.00 48.88	
ATOM	6578	CG1	VAL D				201.478	1.00 51.38	D
MOTA	6579	CG2	VAL D	179			200.934	1.00.53.47	D
ATOM	6580	С	VAL D				199.033	1.00 54.75	D
ATOM	6581	0	VAL D				199.447	1.00 54.64	D
MOTA	6582	N	PRO D				197.877	1.00 54.47	D
ATOM	6583	CD	PRO D				197.133	1.00 50.08	D
ATOM	6584	CA	PRO D				197.048	1.00 50.07	D
ATOM	6585	CB	PRO D				195.653	1.00 46.59	D
ATOM	6586	CG	PRO D	180		108.930		1.00 53.44	D
MOTA	6587	С	PRO D			108.586		1.00 44.18	D
ATOM	6588	0	PRO D			107.753		1.00 36.61	D
ATOM	6589	N	ILE D			108.466		1.00 45.45	D
MOTA	6590	CA	ILE D				198.045	1.00 43.31	D
ATOM	6591	СВ	ILE D				198.974	1.00 44.06	ם מ
ATOM	6592		ILE D			106.459		1.00 49.15	D
ATOM	6593		ILE D				200.097	1.00 44.53	ā
ATOM	6594		ILE D			109.093	-	1.00 42.19	, <u>D</u>
ATOM	6595	С	ILE D			106.480		1.00 44.63	D
ATOM	6596	ō	ILE D			106.863		1.00 40.53	Ď
ATOM	6597	N	PRO D				196.679	1.00 47.10	D
ATOM	6598	CD	PRO D			104.733		1.00 47.00	D
ATOM	6599	CA	PRO D			104.417		1.00 45.23	D
ATOM	6600	CB	PRO D			103.296		1.00 48.60	D
ATOM	6601	CG	PRO D			103.914		1.00 50.26	D
ATOM	6602	C	PRO D			103.912		1.00 45.36	Ď
MOTA	6603	0	PRO D	182		103.247		1.00 43.34	D
ATOM	6604	N	LEU D	183		104.261		1.00 47.19	D
MOTA	6605	CA	LEU D	183		103.815		1.00 47.33	D
MOTA	6606	CB	LEU D	183	87.220	104.592	196.604	1.00 47.21	D
ATOM	6607	CG	LEU D	183	86.108	103.891	197.401	1.00 43.68	D
MOTA	6608	CD1	LEU D				198.568	1.00 43.88	D
ATOM	6609	CD2	LEU D	183	84.931	103,609	196.506	1.00 48.99	D
MOTA	6610	C	LEU D	183	87.080	104.034	194.163	1.00 48.03	D
ATOM	6611	0	LEU D			105.168		1.00 47.91	D.
ATOM	6612	N	THR D	184	86.670	102.929	193.559	1.00 48.10	D
MOTA	6613	CA	THR D	184		102.969		1.00 46.87	D
ATOM	6614	CB	THR D			102.408		1.00 47.03	D
ATOM	6615		THR D			101.185		1.00 52.02	D
ATOM	6616		THR D			103.402		1.00 44.12	D
ATOM	6617	C	THR D			102.114		1.00 45.63	Ď
MOTA	6618	0	THR D			101.353		1.00 43.56	Ď
ATOM	6619	N	VAL D			102.258		1.00 44.30	D
ATOM	6620	CA	VAL D			101.478		1.00 49.34	Ď
ATOM	6621	CB	VAL D	185		102.252		1.00 50.55	Ď

MOTA	6622	CG1	VAL	D 18	5 81.619	102.549	193.690	1.00	60.81	D
ATOM	6623	CG2	VAL	D 18	5 81.065	103.546	191.506	1.00	49.78	D
MOTA	6624	C	VAL	D 18	5 82.108	101.118	190.215	1.00	50.78	D
MOTA	6625	0	VAL	D 18	5 82.223	101.937	189.295	1.00	47.23	D
ATOM	6626	N	TYR	D 18	6 81.650	99.886	190.040	1.00	51.36	D
MOTA	6627	CA	TYR :	D 18	6 81.170		188.739	1.00	52.75	D
MOTA	6628	CB	TYR :	D 18	6 82.181	98.558	188.028	1.00	48.03	D
ATOM	6629	CG	TYR :	D 18	6 82.475	97.282	188.740	1.00	53.26	D
MOTA	6630	CD1	TYR :	D 18	6 81.726	96.127	188.488	1.00	56.60	D
ATOM	6631	CE1				94.945	189.184	1.00	58.09	D
ATOM	6632	CD2	TYR				189.701		60.85	D
MOTA	.6633	CE2	TYR :	D 18	6 83.743		190.410		62.27	D
MOTA	6634	CZ	TYR :	D 18	6 82.985		190.149	1.00	60.16	Ď
ATOM	6635	OH	TYR :	D 18	6 83.214	93.769	190.879		61.60	D
ATOM	6636	С	TYR :	D 18	6 79.863	98.752	188.994		51.88	D
MOTA	6637	0	TYR	D 18	6 79.628	98.252	190.094		48.23	D
MOTA	6638	N	CYS :	D 18	7 79.002	98.755	187.984		54.13	D
ATOM	6639	CA	CYS	D 18	7 77.700	98.118	188.066		53.47	D
MOTA	6640	С	CYS	D 18	7 77.487	97.204	186.864		52.95	D
ATOM	6641	0	CYS	0 18	7 77.680		185.722		50.10	D
MOTA	6642	CB	CYS I	D 18	7 76.588	99.167	188.052		52.28	D
ATOM	6643	SG	CYS	D 18	7 76.703	100.528	189.251	1.00	56.87	D
MOTA	6644	N	ALA I	D 18			187.115	1.00	54.58	D
MOTA	6645	CA	ALA I	D 18	8 76.790	95.023	186.028	1.00	50.96	D
ATOM	6646	CB	ALA I	18	8 76.277	93.714	186.590		47.13	D
MOTA	6647	С	ALA I	18	8 75.763		185.077	1.00	48.42	. Б
MOTA	6648	0	ALA I	18	8 75.778	95.382	183.879	1.00	53.31	a
ATOM	6649	N	LYS I	18	9 74.884	96.467	185.624	1.00	45.53	D
MOTA	6650	CA	LYS I	18	9 73.870	97.155	184.841	1.00	48.59	a
MOTA	6651	CB	LYS I	D 18	9 . 72.465	96.697	185.240	1.00	52.59	. D
MOTA	6652	CG	LYS I	18	9 72.240	95.190	185.223	1.00	55.87	D
MOTA	6653	CD	LYS I	18	9 72.335	94.639	183.815	1.00	59.78	D
ATOM	6654	CE	LYS	18	9 71.318	95.288	182.880	1.00	57.69	D
ATOM	6655	NZ	LYS I	D 18	9 71.566	94.886	181.463	1.00	57.35	D
MOTA	6656	С	LYS I	D 18	9 74.006	98.639	185.162	1.00	52.27	D
ATOM	6657	0	LYS I	18	9 73.936	99.034	186.328	1.00	57.31	D
MOTA	6658	N	SER I	19	0 74.204	99.465	184.144	1.00	50.63	D
ATOM	6659	CA	SER :	19	0 74.334	100.897	184.376	1.00	50.46	D
MOTA	6660	CB	SER :	D 19	0 74.429	101.659	183.057	1.00	52.80	D
MOTA	6661	OG	SER :	D 19	0 73.743	102.903	183.159	1.00	58.11	a
MOTA	6662	С	SER :	0 19	0 73.161	101.449	185.174	1.00	47.62	D
MOTA	6663	0	SER :	D 19	0 72.020	101.039	184.982	1.00	46.56	D
MOTA	6664	N	GLN :	D 19	1 73.462	102.394	186.062	1.00	48.86	D
MOTA	6665	CA	GLN :	0 19	1 72.452	103.035	186.904	1.00	44.46	D
MOTA	6666	CB	GLN :	D 19	1 71.924	102.041	187.927	1.00	41.08	D
MOTA	6667	CG	GLN :	D 19	1 73.006	101.393	188.755		47.69	D
MOTA	6668	CD	GLN :			100.371			48.18	D
ATOM	6669	OE1				100.705	190.605		54.87	D
MOTA	6670	NE2	GLN :			99.113	189.525	1.00	49.21	D
MOTA	6671	C	GLN :			104.250		1.00	41.09	D
MOTA	6672	0	GLN :			104.365			39.13	D
MOTA	6673	N	ASN :			105.160	188.032	1.00	43.34	D
MOTA	6674	CA ·	ASN :			106.353	188.733	1.00	44.26	D
MOTA	6675	CB	ASN :			107.440	188.602		46.27	D
MOTA	6676	CG	ASN :			107.673	187.173	1.00	56.10	D
MOTA	6677		ASN :			107.720			58.79	D
MOTA	6678		ASN :			107.824			62.26	D
ATOM	6679	С	ASN :	D 19	2 72.901	106.111	190.203	1.00	44.03	D

MOTA	6680	0	ASN D	192	72.087	105.564	190.947	1.00 50.24	D
MOTA	6681	N	LEU D	193	74.084	106.527	190.618	1.00 40.97	D
ATOM	6682	CA	LEU D	193	74.505	106.374	191.988	1.00 33.39	D
ATOM	6683	CB	LEU D	193	75.758	105.505	192.080	1.00 29.92	D
ATOM	6684	CG	LEU D	193	75.630	103.998	191.907	1.00 35.43	D
ATOM	6685	CD1	LEU D	193	76.978	103.334	192.199	1.00 26.14	D
ATOM	6686		LEU D		74.555	103.468	192.854	1.00 37.81	D
ATOM	6687	C	LEU D				192.567	1.00 33.85	D
ATOM	6688	Ō	LEU D				191.858	1.00 33.86	D
ATOM	6689	N	GLY D				193.884	1.00 37.65	D
ATOM	6690	CA	GLY D				194.597	1.00 36.81	D
ATOM	6691	C	GLY D				195.891	1.00 35.13	D
ATOM	6692	ō	GLY D				196.275	1.00 33.13	D
ATOM	6693	N	TYR D				196.555	1.00 32.62	D
ATOM	6694	CA	TYR D				197.831	1.00 32.02	
ATOM	6695	CB	TYR D				197.647	1.00 30.68	D
ATOM	6696	CG	TYR D			109.165			D
								1.00 42.29	D
ATOM	6697		TYR D				196.076 195.816	1.00 43.06	D
ATOM	6698	CE1						1.00 44.89	D
MOTA	6699	CD2	TYR D			109.552		1.00 41.41	D
ATOM	6700	CE2	TYR D				198.112	1.00 41.35	- D
MOTA	6701	CZ	TYR D			110.950		1.00 45.25	D
ATOM		OH	TYR D			111.855		1.00 46.12	D
ATOM	6703	C	TYR D				198.805	1.00 29.69	D
MOTA	6704	0	TYR D			111.229		1.00 30.55	D
ATOM	6705	N	TYR D				200.074	1.00 29.95	D
ATOM	6706	CA	TYR D			110.701		1.00 29.48	D
ATOM	6707	CB	TYR D			111.262		1.00 28.82	D
MOTA	6708	CG	TYR D			110.296		1.00 31.05	D
MOTA	6709	CD1				109.802		1.00 32.72	D
ATOM	6710	CE1					204.364	1.00 25.73	D
MOTA	6711	CD2	TYR D			109.880		1.00 24.61	D
MOTA	6712	CE2				109.000		1.00 31.65	D
MOTA	6713	CZ	TYR D			108.523		1.00 32.37	D
MOTA	6714	OH	TYR D			107.662		1.00 29.82	D
ATOM	6715	C	TYR D			110.054		1.00 26.69	D
ATOM	6716	0	TYR D			108.829		1.00 22.17	D
MOTA	6717	N	LEU D			110.895		1.00 26.36	D
ATOM	6718	CA	LEU D			110.478		1.00 22.65	D
MOTA	6719	CB	LEU D			111.329		1.00 21.09	D
MOTA	6720	CG	LEU D			111.225 112.094		1.00 25.29	D
MOTA	6721	CD1	LEU D					1.00 26.86	D
MOTA	6722		LEU D			109.776		1.00 23.27	D
MOTA	6723	C					205.361	1.00 21.12	D
MOTA	6724	0	LEU D SER D			111.369		1.00 21.33	D
MOTA	6725	Ŋ			-	109.874 109.873		1.00 18.32	D
MOTA	6726	CA	SER D			109.873		1.00 18.41	D
MOTA	6727	CB	SER D			107.536		1.00 19.24 1.00 26.22	D
MOTA	6728	OG				107.538			D
ATOM	6729	C	SER D			109.518		1.00 20.67 1.00 14.54	D
MOTA	6730	0					208.545		D
MOTA	6731	N		199 ·				1.00 22.31	D
MOTA	6732	CA	GLY D			109.926		1.00 18.29	D
MOTA	6733	C	GLY D			111.126		1.00 21.63	D
ATOM	6734	0	GLY D			112.187		1.00 25.72	D
MOTA	6735	N	THR D			110.953		1.00 27.65	D
ATOM	6736	CA	THR D			112.019		1.00 28.35	D
MOTA	6737	CB	THR D	200	82.337	111.4/6	215.246	1.00 26.26	D

MOTA	6738	OG1	THR	D	200	81.558	110.383	215.724	1.00	24.88	D
ATOM	6739	CG2	THR	D	200	82.408	112.541	216.309	1.00	26.91	D
MOTA	6740	C	THR					213.437		26.16	D
ATOM	6741	0	THR					212.948		25.10	Ď
ATOM	6742	N	THR	_				213.538		26.66	Ď
ATOM	6743	CA	THR				_	213.017		28.27	Ď
ATOM	6744	CB	THR				· · · · · -	212.085			
ATOM	6745	OG1						212.003		25.56	D
ATOM		CG2	THR							25.73	D
	6746							212.257		32.55	D
MOTA	6747	C	THR					214.100		29.04	D
ATOM	6748	0	THR					215.224		30.68	D
MOTA	6749	N	ALA					213.761		23.57	D
MOTA	6750	CA	ALA					214.762	1.00	25.46	D
MOTA	6751	CB	ALA	D	202	86.361	117.754	214.971	1.00	18.10	D
MOTA	6752	С	ALA			84.741	119.601	214.468	1.00	26.45	D
MOTA	6753	0	ALA	D	202	85.314	120.431	215.185	1.00	27.35	D
ATOM	6754	N	ASP :			83.975	119.949	213.445	1.00	25.29	D
MOTA	6755	CA	ASP :	D	203	83.859	121.355	213.067	1.00	22.97	D
ATOM	6756	CB	ASP :	D	203	84.751	121.632	211.865	1.00	26.02	D
MOTA	6757	CG	ASP :					210.692	1.00	31.30	D
MOTA	6758	OD1	ASP :	D	203			209.563	1.00		D
ATOM	6759	_	ASP	_				210.892		35.08	D
ATOM	6760	C	ASP :					212.720		23.55	D
ATOM	6761	ō	ASP :					212.423	1.00		D
ATOM	6762	N	ALA					212.747	1.00		
ATOM	6763	CA	ALA					212.747			D
ATOM	6764	CB	ALA :							22.77	D
								212.701		12.66	D
ATOM	6765	C	ALA :					210.964		28.34	. D
ATOM	6766	0	ALA I					210.620		34.32	. D
ATOM	6767	N	GLY :					210.107		27.24	D
ATOM	6768	CA	GLY :					208.703		30.80	D
MOTA	6769	C	GLY :					208.514		31.29	D
ATOM	6770	0	GLY :					207.413	1.00	28.93	D
ATOM	6771	N	ASN :			81.100	120.781	209.622	1.00	33.30	Ď
ATOM	6772	CA	ASN :	D	206	80.833	119.359	209.634	1.00	34.62	D
ATOM	6773	CB	ASN :	D	206	79.314	119.141	209.528	1.00	34.30	D
ATOM	6774	CG	ASN 1	D	206	78.914	117.693	209.726	1.00	41.52	D
ATOM	6775	OD1	ASN :	D	206	78.180	117.127	208.916	1.00	46.41	D
MOTA	6776	ND2	ASN :	D	206	79.390	117.084	210.806	1.00	37.73	D
ATOM	6777	C	ASN :	D	206	81.577	118.566	208.558	1.00	31.76	D
MOTA	6778	0	ASN :	D	206	81.035	117.626	207.997	1.00	33.42	D
ATOM	6779	N	SER :	D	207	82.830	118.918	208.289	1.00	32.35	D
ATOM	6780	CA	SER :	D	207	83.582	118.188	207.268	1.00	31.44	D
ATOM	6781	CB	SER :	D	207			205.993		30.73	D
ATOM	6782	OG	SER :				119.981			36.30	D
ATOM	6783	C	SER				117.728			30.24	Ď
ATOM	6784	ō	SER				117.320			33.61	D
ATOM	6785	N	ILE :				117.801			29.94	D
ATOM	6786	CA	ILE :				117.342			28.43	
ATOM	6787	CB	ILE :				118.475			21.19	D
ATOM	6788		ILE :				118.000				D
										16.12	D
ATOM	6789		ILE :				119.649	-		21.74	D
ATOM	6790		IFE :				120.928			23.38	D
ATOM	6791	C	ILE :				116.199			32.84	D
ATOM	6792	0	ILE !				116.412			35.66	ם
ATOM	6793	N	PHE				114.980			34.36	D
MOTA	6794	CA	PHE :				113.826			36.28	D
ATOM	6795	CB	PHE :	D	209	86.291	112.561	209.956	1.00	33.39	D

MOTA	6796	CG	PHE	D 209	85.113	112.542	209.018	1.00 30.28	D
MOTA	6797	CD1	PHE	D 209	85.184	113.171	207.779	1.00 30.91	. Б
MOTA	6798		PHE			112.004		1.00 34.03	D
ATOM	6799								
			PHE			113.276		1.00 32.18	D
ATOM	6800		PHE :			112.101		1.00 35.54	D
ATOM	6801	cz	PHE :	D 209	82.833	112.743	207.384	1.00 35.20	D
ATOM	6802	C	PHE :	209	87.268	113.639	212.002	1.00 41.75	D
ATOM	6803	0	PHE :			113.514		1.00 49.71	. Д
ATOM	6804	N		0 210		113.647		1.00 45.28	D
ATOM									
	6805	CA		210		113.490		1.00 47.85	D
ATOM	6806	CB		210		113.139		1.00 48.72	D
ATOM	6807	OG1				114.307		1.00 53.11	D
MOTA	6808	CG2	THR :	D 210	86.871	112.610	216.785	1.00 52.44	D
MOTA	6809	C	THR :	D 210	88.387	112.438	214.516	1.00 50.24	D
ATOM	6810	0	THR :	210	88.252	111.361	213.941	1.00 47.20	D
ATOM	6811	N	ASN I	211	89.469	112.758	215.227	1.00 55.04	D
ATOM	6812	CA	ASN :			111.824		1.00 56.56	D
ATOM	6813	CB	ASN I			112.514	-	1.00 58.25	ā
			ASN I			111.537			
MOTA	6814	CG						1.00 60.84	D
ATOM	6815	OD1				111.926		1.00 66.22	D
ATOM	6816		ASN I	-		110.264		1.00 54.74	, D
ATOM	6817,	C	ASN I	211	90.211	110.744	216.356	1.00 56.12	D
MOTA	6818'	0	ASN I	211	90.004	111.006	217.530	1.00 54.01	D
MOTA	6819	N	THR !	212	90.157	109.521	215.862	1.00 60.18	D
ATOM	6820	CA	THR 1			108.367		1.00 63.67	D
ATOM	6821	CB		212		107.628		1.00 61.63	D
ATOM	6822	OG1				108.359		1.00 58.04	Ď
		CG2							
ATOM	6823					106.212		1.00 65.60	D
MOTA	6824	C		212		107.430		1.00 68.00	D
ATOM	6825	0		212	91.345	106.737	215.792	1.00 68.19	D
MOTA	6826	N	ALA 1	213		107.413		1.00 71.03	D
ATOM	6827	CA	ALA 1	213	92.838	106.566	218.111	1.00 73.96	D
MOTA	6828	CB	ALA I	213	93.956	106.985	217.171	1.00 68.36	D
ATOM	6829	C	ALA I	213	93.291	106.699	219.552	1.00 78.61	D
ATOM	6830	ō	ALA I			107.717		1.00 75.31	Ď
ATOM	6831	N		214		105.670		1.00 85.62	Ď
ATOM	6832	CA		214		105.686		1.00 92.04	D
ATOM	6833	CB		214		104.309		1.00 91.32	Ď
MOTA	6834	OG		214		104.390		1.00 96.07	D
MOTA	6835	C	SER 1	214	95.927	106.131	221.522	1.00 96.25	D
ATOM	6836	0	SER I	214	96.210	107.173	222.124	1.00 94.70	D
MOTA	6837	N	PHE 1	215	96.847	105.364	220.931	1.00100.55	D
MOTA	6838	CA	PHE I	215	98.278	105.695	220.987	1.00106.21	D
ATOM	6839	CB		215		104.976		1.00114.06	D
ATOM	6840	CG		215		105.265		1.00122.71	D
ATOM	6841	-	PHE			105.226		1.00125.55	D
			PHE			105.578		1.00123.33	·
MOTA	6842								D _.
MOTA	6843		PHE !			105.499		1.00126.25	D
MOTA	6844		PHE 1			105.850		1.00125.01	D
ATOM	6845	CZ		215		105.811		1.00126.05	D
MOTA	6846	С		215		107.195		1.00105.82	D
MOTA	6847	0	PHE I	215	98.679	107.752	219.794	1.00103.54	D
ATOM	6848	N		216		107.825		1.00106.12	ם
ATOM	6849	CA	SER			109.253		1.00105.35	D
MOTA	6850	CB	SER I			109.519		1.00103.35	D
ATOM	6851	OG	SER I			110.887			
								1.00109.15	D
MOTA	6852	C		216	98.324	109.965	220.986	1.00103.14	D
ATOM	6853	. 0	SER	216	98.916	110.174	219.925	1.00104.74	D

MOTA	6854	N	PRO	D	217	97.060	110.349	221.183	1.00	99.73	D
MOTA	6855	CD	PRO	D	217	96.344	110.325	222.469	1.00	99.02	D
MOTA	6856	CA	PRO	D	217	96.269	111.041	220.166	1.00	96.62	D
MOTA	6857	CB	PRO	D	217	94.924	111.237	220.859	1.00	98.45	D
MOTA	6858	CG	PRO	D	217	95.329	111.431	222.284	1.00	98.16	D
MOTA	6859	C .	PRO	D	217	96.857	112.361	219.694	1.00	90.70	D
ATOM	6860	0	PRO	D	217	96.718	113.378	220.369	1.00	89.52	D
ATOM	6861	N	ALA	D	218		112.339			83.37	D
ATOM	6862	CA	ALA	D	218		113.561			79.95	D
ATOM	6863	CB	ALA				113.324			77.78	D
ATOM	6864	C	ALA				114.531	_		78.09	D
MOTA	6865	ō	ALA				114.611			83.21	D
MOTA	6866	N	GLN		-		115.259			72.86	D
ATOM	6867	CA	GLN				116.194			71.16	D
MOTA	6868	CB	GLN				116.715	_		73.68	. D
ATOM	6869	CG	GLN			-	117.709			81.65	D
MOTA	6870	CD	GLN				118.381			87.94	D.
ATOM	6871	OE1	GLN				119.222			91.13	D
MOTA	6872	NE2	GLN				118.015			92.41	D
ATOM	6873	C	GLN				117.390			67.43	D
MOTA	6874	ŏ	GLN				117.791			65.06	D
ATOM	6875	N	GLY	_			117.950			66.01	D
ATOM	6876	CA	GLY				119.133			63.87	D
ATOM	6877	C	GLY				118.993			61.04	D
ATOM	6878	ō	GLY				119.994			58.72	D
ATOM	6879	N	VAL				117.774			57.83	ם
ATOM	6880	CA	VAL				117.585			54.92	D
MOTA	6881	CB	VAL				116.701			53.92	D
ATOM	6882		VAL				116.889			53.17	D
ATOM	6883	CG2	VAL				117.059			50.61	ā
ATOM	6884	C	VAL				117.014			54.08	D D
ATOM	6885	ō	VAL				117.595			55.95	D
ATOM	6886	N	GLY				115.885			50.29	D
ATOM	6887	CA	GLY				115.295			45.40	D
ATOM	6888	C	GLY				115.107			39.80	Ď
ATOM	6889	ō	GLY				115.872			41.10	D -
ATOM	6890	N	VAL				114.092			34.73	ā
ATOM	6891	CA	VAL				113.759			32.14	ā
ATOM	6892	CB	VAL					208.442		35.22	D
ATOM	6893		VAL				111.888			34.40	D
ATOM	6894	CG2					111.577			32.82	D
MOTA	6895	C			223		114.384			30.52	D
MOTA	6896	Ō			223		114.339			30.39	D
ATOM	6897	N			224		114.955			29.44	D
MOTA	6898	CA			224		115.577			31.99	D
ATOM	6899	CB	GLN	D	224		117.087			22.25	D
MOTA	6900	CG	GLN	D	224		117.819	_		29.08	D
ATOM	6901	CD			224		119.302			36.59	D
ATOM	6902		GLN				120.150			42.00	D
ATOM	6903		GLN				119.617			39.93	Ď
ATOM	6904	C			224		114.996			35.66	D
ATOM	6905	ō			224		114.856			37.26	D
ATOM	6906	N			225		114.641			35.79	D
ATOM	6907	CA			225		114.050			30.99	D
ATOM	6908	CB			225		112.838			27.28	D
ATOM	6909	CG			225		111.727			33.61	D
ATOM	6910		LEU				110.453				. D
ATOM	6911		LEU			89.004	111.466	203.446		36.51	. D
				_							_

MOTA	6912	C	LEU I	225		87.804	115.054	201.394	1.00	31.00	D
ATOM	6913	0	LEU I	225		86.932	115.917	201.551	1.00	32.09	D
ATOM	6914	N		226				200.276		28.47	D
ATOM	6915			226							
		CA						199.187		25.76	D
MOTA	6916	CB		226			116.780		1.00	23.32	D
MOTA	6917	OG1	THR I	226		89.146	118.041	198.642	1.00	29.32	D
ATOM	6918	CG2	THR I	226		90.675	116.154	198.478	1.00	18.21	D
MOTA	6919	C	ז מאד	226				197.866		25.30	D
ATOM	6920	ō		226			113.919				
										20.99	D
MOTA	6921	N	ARG I				115.591			26.38	D
MOTA	6922	CA	ARG I	227		37.172	114.946	195.618	1.00	31.47	D
MOTA	6923	CB	ARG I	227	1	35.683	114.524	195.425	1.00	23.83	D
MOTA	6924	CG	ARG I	227	1	34.663	115.657	195.516	1.00	22.21	D
MOTA	6925	CD	ARG I	227			115.165			30.01	D
ATOM	6926	NE	ARG I				116.163			26.28	Ď
ATOM	6927	CZ	ARG I				116.984				
ATOM	6928		ARG I							30.20	D
							116.934			37.40	D
ATOM	6929		ARG I				117.877			29.17	D
MOTA	6930	C	ARG I		8	37.629	115.951	194.549	1.00	33.56	· D
MOTA	6931	0	ARG I				116.904		1.00	26.33	D
MOTA	6932	N	ASN I	228	1	38.847	115.728	194.047	1.00	39.95	D
MOTA	6933	CA	ASN I	228	{	39.469	116.628	193.068	1.00	42.75	D
MOTA	6934	CB	ASN I	228	8	38.761	116.534	191.716		47.73	D
MOTA	6935	CG	ASN I				115.265			56.00	D
ATOM	6936		ASN I				115.171			68.18	
MOTA			ASN I								D
	6937						114.276			55.97	D
ATOM	6938	C	ASN I				118.068			40.30	D
MOTA	6939	0	ASN I				118.982		1.00	39.54	D
MOTA	6940	N	GLY I	229			118.257		1.00	39.42	D
ATOM	6941	CA	GLY I	229	8	39.901	119.587	195.379	1.00	42.64	D
MOTA	6942	С	GLY I	229	8	88.668	120.042	196.141	1.00	44.99	D
MOTA	6943	0	GLY I				120.935			46.97	D
ATOM	6944	N	THR I				119.463			42.99	D
ATOM	6945	CA	THR I				119.855			41.26	
ATOM	6946	CB	THR I								D
							119.573			42.11	D
ATOM	6947		THR I				120.479			43.56	D
MOTA	6948	CG2					119.755		1.00	42.63	D
MOTA	6949	С	THR I	230	8	36.134	119.094	197.826	1.00	43.32	D
ATOM	6950	0	THR I	230	8	36.321	117.872	197.868	1.00	47.88	D
MOTA	6951	N	ILE I	231	{	35.796	119.822	198.883	1.00	36.94	D
ATOM	6952	CA	ILE I	231	8	35.629	119.228	200,195		33.80	D
ATOM	6953	CB	ILE D	231			120.312			38.72	D
ATOM	6954	CG2					119.730			33.72	D.
ATOM	6955			231			120.877				_
ATOM	6956		ILE I							33.42	D
							121.972			39.63	D
ATOM	6957	C	ILE I				118.503			30.75	D
MOTA	6958	0	ILE D				118.964			30.78	D
MOTA	6959	И	ILE D	232	٠ (34.311	117.363	200.940	1.00	28.89	D
MOTA	6960	CA	ILE D	232		33.091	116.596	201.088	1.00	28.70	D
MOTA	6961	CB	ILE D	232			115.145		1.00	28.24	D
ATOM	6962	CG2	ILE I	232			114.361		1.00	22.26	D
MOTA	6963		ILE I				115.146			27.91	D
ATOM	6964	נתי	ILE I	222			113.140			13.19	
MOTA	6965	CDI	ILE I								D
							116.577			29.44	D
MOTA	6966	0	ILE I				115.828			33.08	D
MOTA	6967	N	PRO D				117.448			25.35	D
ATOM	6968	CD	PRO I				118.701			18.19	D
MOTA	6969	CA	PRO D	233	8	31.199	117.418	204.285	1.00	27.11	D

MOTA	6970	CB	PRO D	233		80.463	118.755	204.438	1.00 28	.32	D
MOTA	6971	CG	PRO D	233		80.099	119.131	203.041	1.00 23	.27	D
ATOM	6972	C	PRO D	233		80.274	116.212	204.482	1.00 28	. 07	D
MOTA	6973	0	PRO D	233		79.661	115.730	203.527	1.00 29	.41	D
MOTA	6974	N	ALA D	234		80.191	115.721	205.711	1.00 25	.19	D
ATOM	6975	CA	ALA D	234		79.336	114.577	206.032	1.00 24	.45	D
MOTA	6976	CB	ALA D	234				207.500	1.00 23		D
MOTA	6977	C	ALA D				114.833		1.00 23		D
ATOM	6978	0	ALA D					205.826	1.00 22		D
ATOM	6979	N	ASN D					205.115	1.00 20		D
ATOM	6980	CA	ASN D				113.928		1.00 24		D
-ATOM	6981	CB	ASN D					205.987	1.00 21		D
ATOM	6982	CG	ASN D				113.170		1.00 31		Ď
ATOM	6983		ASN D					208.137	1.00 30		Ď
ATOM	6984		ASN D				111.921		1.00 27		Ď
ATOM	6985	C	ASN D				114.970		1.00 27		Ď
ATOM	6986	ō	ASN D				115.689		1.00 29		D
ATOM	6987	N	ASN D				115.040		1.00 28		Ď
ATOM	6988	CA	ASN D				115.943		1.00 28		Ď
ATOM	6989	CB	ASN D				116.927		1.00 40		Ď
ATOM	6990	CG	ASN D				117.714		1.00 42		Ď
ATOM	6991		ASN D				118.424		1.00 44		D
ATOM	6992		ASN D				117.585		1.00 48		D
ATOM	6993	C	ASN D				114.981		1.00 30		Ď
ATOM	6994	ō	ASN D				114.524		1.00 35		Ď
ATOM	6995	N	THR D		•		114.659		1.00 27.		D
ATOM	6996	CA	THR D				113.692		1.00 29		Ď
ATOM	6997	CB	THR D				113.232		1.00 32		D
ATOM	6998		THR D				112.933		1.00 38.		. D
ATOM	6999	CG2	THR D				111.973		1.00 31.		D
ATOM	7000	C	THR D			•	114.143		1.00 30.		ם
ATOM	7001	ō	THR D				115.179		1.00 30.		D
MOTA	7002	N	VAL D				113.353		1.00 30.		D
ATOM	7003	CA	VAL D				113.632		1.00 34.		Ď
ATOM	7004	CB	VAL D				113.331		1.00 38.		Ď
ATOM	7005	-	VAL D				113.353		1.00 37.		Ď
ATOM	7006		VAL D				114.356		1.00 48.		Ď
ATOM	7007	C	VAL D				112.726		1.00 36.		D
ATOM	7008	ō	VAL D				111.494		1.00 35.		D
ATOM	7009	N	SER D				113.340		1.00 38.		D
ATOM	7010	CA	SER D				112.586		1.00 40.		D
ATOM	7011	CB	SER D				113.427		1.00 43.		D
MOTA	7012	OG	SER D				112.686		1.00 57.		D
ATOM	7013	c	SER D				112.095		1.00 38.		D
ATOM	7014	ō	SER D				112.888	~	1.00 43.		Ď
MOTA	7015	N	LEU D				110.781		1.00 37.		Ď
ATOM	7016	CA	LEU D				110.149		1.00 37.		Ď
MOTA	7017	CB	LEU D				108.754		1.00 30.		Ď
ATOM	7018	CG	LEU D	-			108.698		1.00 30.		D
ATOM	7019		LEU D				107.275		1.00 35.		D
ATOM	7020		LEU D				109.170		1.00 20		D
MOTA	7021	C	LEU D				110.034		1.00 38.		Ď
ATOM	7022	ō	LEU D				109.725		1.00 33.		. D
MOTA	7023	N	GLY D				110.279		1.00 33.		· D
ATOM	7024	CA	GLY D				110.275		1.00 42.		ם
ATOM	7025	C	GLY D				108.701		1.00 44.		Ð
ATOM	7025	ō	GLY D				107.924		1.00 43.	•	D
ATOM	7027	И	ALA D				107.324		1.00 45.		D
	,	**						~~~.	4.00 40.		U

MOTA	7028	CA	ALA D	242	75.504	106.934	185.534	1.00	44.50	D
MOTA	7029	CB	ALA D	242	75.015	106.861	184.119	1.00	44.60	D
MOTA	7030	С	ALA D	242	76.802	106.168	185.669	1.00	44.15	D
ATOM.	7031	0	ALA D	242	77.841	106.599	185.174	1.00	44.58	D
MOTA	7032	N	VAL D	243	76.738	105.039	186.360	1.00	44.23	D
MOTA	7033	CA	VAL D	243	77.903	104.199	186.556	1.00	46.51	D
ATOM	7034	CB	VAL D	243	78.184	103.981	188.038	1.00	43.76	D
MOTA	7035	CG1	VAL D	243	79.424	103.115	188.212	1.00	43.46	D
ATOM	7036	CG2	VAL D	243	78.362	105.313	188.710	1.00	50.13	D
MOTA	7037	C	VAL D	243	77.590	102.861	185.903	1.00	. 49.53	D
MOTA	7038	0	VAL D	243	76.536	102.272	186.158	1.00	53.02	D
MOTA	7039	N	GLY D	244	78.505	102.391	185.062	1.00	45.58	D
MOTA	7040	CA	GLY D	244	78.290	101.140	184.379	1.00	43.81	D
MOTA	7041	C	GLY D	244	79.364	100.095	184.580	1.00	47.30	ם
MOTA	7042	0	GLY D	244	79.917	99.938	185.676	1.00	47.49	D
MOTA	7043	N	THR D	245	79.666	99.381	183.500	1.00	50.57	D
MOTA	7044	CA	THR D	245	80.642	98.299	183.534	1.00	51.81	D
ATOM	7045	CB	THR D	245	80.520	97.424	182.260	1.00	51.13	D
ATOM	7046	OG1	THR D	245	80.552	98.253	181.090	1.00	55.23	D
MOTA	7047	CG2	THR D	245	79.200	96.661	182.284	1.00	46.04	D
MOTA	7048	C	THR D	·245	82.073	98.756	183.742	1.00	50.91	D
MOTA	7049	0	THR D	245	82.905	98.003	184.253	1.00	53.14	D
ATOM	7050	N	SER D	246	82.359	99.993	183.352	1.00	51.11	D
ATOM	7051	CA	SER D	246		100.550		1.00	50.38	D
ATOM	7052	CB	SER D	246	84.020	101.577	182.452	1.00	49.82	D
ATOM	7053	OG	SER D	246	83.704	101.083	181.165	1.00	57.34	D
ATOM	7054	C	SER D	246 .	83.681	101.244	184.895	1.00	47.94	D
ATOM	7055	0	SER D	246		102.103		1.00	47.72	D
ATOM	7056	N	ALA D		84.611	100.861	185.760	1.00	44.78	D
MOTA	7057	CA	ALA D	247		101.449		1.00	45.33	D
MOTA	7058	CB	ALA D		85.910	100.866	187.815	1.00	44.79	D
ATOM	7059	С	ALA D	247	84.827	102.974	187.041	1.00	46.03	D
MOTA	7060	0	ALA D		85.380	103.550	186.108	1.00	48.87	D
ATOM	7061	N	VAL D			103.621	188.058	1.00	44.62	D
MOTA	7062	CA	VAL D				188.156	1.00	45.32	D
ATOM	7063	CB	VAL D			105.677			46.30	D
MOTA	7064		VAL D			107.153			42.83	D
ATOM	7065		VAL D			105.485			44.21	D
ATOM	7066	C	VAL D			105.394			48.91	D
ATOM	7067	0	VAL D			104.931	•		51.75	D
ATOM	7068	N	SER D			106.191			48.11	D
MOTA	7069	CA	SER D			106.602			45.35	. D
ATOM	7070	CB	SER D			107.022			42.10	D
ATOM	7071	OG	SER D			107.301			39.95	D
ATOM	7072	C	SER D			107.780			44.60	D
ATOM	7073	0	SER D			108.708			42.89	D
ATOM	7074	N	TEA D			107.744			45.11	D
ATOM	7075	CA	LEU D			108.868			46.11	D
ATOM	7076	CB	LEU D			108.490			48.42	D
ATOM	7077	CG	LEU D			107.277			51.17	D
MOTA	7078		LEU D			107.308			46.15	D
ATOM	7079		TEA D			107.303			45.53	D
ATOM	7080	C	LEU D			110.032			45.02	D
ATOM	7081	0	LEU D			111.171	•		41.99	D
ATOM	7082	N	GLY D			109.726			39.63	D
MOTA	7083	CA	GLY D			110.741			39.22	D
ATOM	7084	C	GLY D			111.335			39.04	D
ATOM	7085	0	GLY D	45±	88.757	112.560	174.5/4	T.00	43.58	D

MOTA	7086	N	LEU	D	252	88.871	110.458	195.385	1.00	34.35	D
ATOM	7087	CA	LEU	D	252	88.999	110.878	196.765	1.00	36.45	D
MOTA	7088	CB	LEU	D	252			197.688		35.74	D
ATOM	7089	CG	LEU	D	252			197.565		31.39	D
MOTA	7090	CD1						198.451		28.23	D
ATOM	7091							197.949		27.38	D
ATOM	7092	C	LEU					197.227		35.68	
ATOM	7093	Ö	LEU		-						D
ATOM		И						196.764		40.05	D _
	7094		THR					198.150		34.52	D
ATOM	7095	CA	THR					198.743		35.10	D
ATOM	7096	CB	THR		_			198.142		37.63	D
ATOM	7097	OG1						196.950		42.09	D
ATOM	7098	CG2	THR					199.128		24.76	D
ATOM	7099	C	THR					200.210		35.90	D
MOTA	7100	0	THR			90.820	113.226	200.569		34.87	D
ATOM	7101	N	ALA	D	254			201.056	1.00	31.41	D
ATOM	7102	CA	ALA	D	254	92.454	112.069	202.490	1.00	32.89	D
MOTA	7103	CB	ALA	D	254	92.915	110.841	203.274	1.00	22.29	D
MOTA	7104	C	ALA	D	254	93.367	113.272	202.787	1.00	38.15	D
MOTA	7105	0	ALA	D	254	94.504	113.350	202.306	1.00	40.40	D
ATOM	7106	N	ASN	D	255		114.210			39.54	D
MOTA	7107	CA	ASN	D	255	93.601	115.409	203.938		38.37	D
ATOM	7108	CB	ASN				116.634			32.80	D
ATOM	7109	CG	ASN				116.529			31.80	. D
ATOM	7110	-	ASN				117.044			36.08	D
ATOM	7111		ASN				115.862			39.71	D
ATOM	7112	C	ASN				115.627			38.87	D.
ATOM	7113	ō	ASN				115.278			42.12	
ATOM	7114	N	TYR				116.207			39.04	D
ATOM	7115	CA	TYR				116.539			36.05	D
ATOM	7116	CB	TYR				116.533				
ATOM	7117	CG	TYR				115.202			32.41	D
ATOM			TYR							29.12	, D
ATOM	7118 7119		TYR :				114.847			28.62	D
ATOM							113.668			31.66	D
	7120	CD2	TYR :				114.332			28.02	D
ATOM	7121	CE2	TYR :				113.143			32.95	D
MOTA	7122	CZ	TYR :				112.813			37.34	D
ATOM	7123	OH	TYR :				111.643			30.52	D
ATOM	7124	C	TYR :				117.969			35.46	D
MOTA	7125	0	TYR :				118.813			37.11	D
MOTA	7126	N	ALA :				118.231			35.88	D
MOTA	7127	CA	ALA :				119.564			36.41	D
MOTA	7128	CB	ALA :				119.585			35.53	D
ATOM	7129	C	ALA :				119.856			41.40	D
ATOM	7130	0	ALA :				118.940			41.85	D
MOTA	7131	N	ARG :					210.438			D
MOTA	7132	CA	ARG :				121.461			53.13	D
MOTA	7133	CB	ARG :				122.688		1.00	57.05	D
MOTA	7134	CG	ARG :			95.267	122.482	211.604	1.00	59.44	D
ATOM	7135	CD	ARG :	D	258	96.005	123.794	211.712	1.00	70.48	D
MOTA	7136	NE	ARG :	D	258	95.959	124.318	213.075	1.00	79.47	D
MOTA	7137	CZ	ARG :	D	258	96.187	125.588	213.393	1.00	83.17	D
MOTA	7138	NH1	ARG :	D	258	96.471	126.469	212.442	1.00	86.75	D
ATOM	7139		ARG I				125.978			86.31	D
MOTA	7140	С	ARG :				121.733			53.99	D
MOTA	7141	0	ARG :				122.467			53.11	D
MOTA	7142	N	THR				121.140			54.62	D
ATOM	7143	CA	THR				121.283			57.01	D
		_									

MOTA	7144	CB	THR	D	259	8	9.868	120	.037	215.231	1.00	56.62	D
ATOM	7145	OG1	THR	D	259	9:	1.048	119	.673	215.956	1.00	63.13	D
MOTA	7146	CG2	THR	D	259	89	9.469	118	.896	214.336	1.00	62.99	D
MOTA	7147	С	THR	D	259	90	0.234	122	.445	215.366	1.00	60.43	D
ATOM	7148	0	THR	D	259	89	9.789	123	.551	215.058	1.00	58.62	D
ATOM	7149	N	GLY	D	260	90	0.823	122	.169	216.529		66.46	D
ATOM	7150	CA	GLY							217.571		69.32	D
MOTA	7151	С	GLY							217.254		70.64	D
ATOM	7152	0	GLY							216.324		70.48	D
ATOM	7153	N	GLY							218.026		73.69	D
ATOM	7154	CA	GLY							217.791		75.92	D
ATOM	7155	C	GLY							217.747		77.22	ā
ATOM	7156	ō	GLY							216.671		78.84	D
ATOM	7157	N	GLN							218.916		76.59	Ď
ATOM	7158	CA	GLN							218.997		77.05	D
ATOM	7159	CB	GLN	_						220.448		85.73	Ď
ATOM	7160	CG	GLN							220.649		93.06	D
ATOM	7161	CD	GLN							220.326		97.67	ă
ATOM	7162		GLN							220.926		99.48	. D
ATOM	7163	NE2	GLN							219.367		99.46	Ď
ATOM	7164	C	GLN							218.501		72.22	Ď
ATOM	7165	ō	GLN							219.057		72.19	ם
ATOM	7166		VAL							217.454		65.55	D.
	7167	CA	VAL							216.926		60.92	D
ATOM	7168	CB	VAL							215.460		56.60	ם
ATOM	7169		VAL							214.967		55.29	D
ATOM	7170		VAL							214.579		47.68	D.
ATOM	7171	C	VAL							217.812		60.13	. D
ATOM	7172	o	VAL							218.351		64.49	
ATOM	7173	N	THR							217.959			D
ATOM	7174	CA	THR									58.39	ם
	7175	CB	THR							218.827 220.169		59.70	D
ATOM	7176	OG1	THR									56.54	D
MOTA	7177	CG2	THR							220.647 221.155		55.52	D
ATOM ·	7178	CGZ	THR									46.38	D
ATOM.	7179		THR							218.278		68.00	D
ATOM	7180	N O	ALA	-	_					217.634		72.49	D
ATOM	7181		ALA							218.539		71.03	D
		CA								218.050		72.38	D
ATOM	7182	CB	ALA		265.					218.482		75.56	D
ATOM	7183	G		_						218.521		73.65	D
ATOM	7184	0	ALA							219.540		75.04	D
MOTA	7185	N	GLY							217.764		74.97	D
ATOM	7186	CA	GLY							218.098		73.80	D
MOTA	7187	C	GLY							216.890		72.02	D
ATOM	7188	0	GLY							215.757		71.30	D
ATOM	7189	N	ASN							217.125		70.32	D
ATOM	7190	CA	ASN							216.039		69.49	D
MOTA	7191	CB	ASN							216.367		74.05	D
ATOM	7192	CG	ASN							216.191		78.81	D
ATOM	7193		ASN							216.367		77.68	D
ATOM	7194		ASN							215.835		80.93	D
MOTA	7195	C	ASN							215.700		65.66	D
ATOM	7196	0	ASN					-		216.541		59.57	D
ATOM	7197	N	VAL							214.443		62.93	D
MOTA	7198	CA	VAL							213.941		60.04	D
ATOM	7199	CB	VAL							213.003		59.12	D
MOTA	7200		VAL							212.454		59.32	D
ATOM	7201	CG2	VAL	D	268	96	.706	112	.545	213.757	1.00	64.04	D

MOTA	7202	С	VAL :	D 26	68			109.121			1.00	59.11	D
MOTA	7203	0	VAL :	D 20	68	95.55	50	108.724	212	.094	1.00	57.26	D
ATOM	7204	N	GLN :	D 26	59	94.02	22	108.595	213	.733	1.00	59.62	D
MOTA	7205	CA	GLN :			93.27	76	107.528	213	.095	1.00	64.07	D
ATOM	7206	CB	GLN :			93.40	7	106.245	213	.916	1.00	66.32	D
MOTA	7207	CG	GLN :	D 26	59	94.71	L7	105.503	213	.716	1.00	69.36	D
MOTA	7208	CD	GLN :	D 26	59	94.90	00	104.367	214	.711	1.00	75.58	D
MOTA	7209	OE1	GLN :					103.567			1.00	78.64	D
MOTA	7210	NE2				96.08	37	104.286	215	.304	1.00	79.82	D
MOTA	7211	C	GLN :	D 26	59	91.80)6	107.925	212	. 939	1.00	66.74	D
ATOM	7212	Ο.	GLN I	D 26	59	91.28	36	108.750	213	. 697	1.00	67.92	D
MOTA	7213	N	SER I	D 27	70	91.13	37	107.356	211	.942	1.00	66.82	D
ATOM	7214	CA	SER I	D 27	70	89.73	9	107.687	211	.727	1.00	64.14	D
MOTA	7215	CB	SER I	D 27	70	89.62	23	109.084	211	.124	1.00	65.34	D
MOTA	7216	OG	SER I	D 2'	70			109.430			1.00	75.40	D
MOTA	7217	С	SER I	D 27	70			106.697			1.00	61.93	D
MOTA	7218	0	SER I	D 21	70	89.50	6	106.045	209	. 967		63.64	D
MOTA	7219	N	ILE 1	D 2	7 1	87.67	70	106.595	211	.178	1.00	58.99	D
MOTA	7220	CA	ILE 1					105.706				53.49	D
MOTA	7221	CB	ILE 1	D 21	71			104.662				56.22	D
ATOM	7222	CG2	ILE 1	D 27	71			103.476				58.72	. D
MOTA	7223	CG1	ILE 1	D 27	71			105.318				58.13	D
ATOM	7224	CD1	ILE 1	D 27	71			104.336				63.90	D
ATOM	7225	C	ILE 1	D 27	71			106.527				47.12	D
ATOM	7226	0	ILE :					107.263				46.02	D
ATOM	7227	N	ILE 1					106.410				41.39	D
ATOM	7228	CA	ILE I		_			107.145				36.85	D
ATOM	7229	CB	ILE I					108.094				36.82	D
ATOM	7230	CG2	ILE I					108.906				35.18	D
ATOM	7231		ILE 1					109.039				49.12	Ď
ATOM	7232		ILE I					109.953				54.29	D
ATOM	7233	C	ILE I					106.211				35.12	D
ATOM	7234	ŏ	ILE I					105.195				36.52	D
ATOM	7235	N	GLY I					106.553				30.16	Ď
ATOM	7236	CA	GLY I					105.719				31.96	D
ATOM	7237	C	GLY I					106.344				34.87	D
ATOM	7238	ō	GLY I					107.568				33.97	Ď
MOTA	7239	N	VAL I					105.514				33.38	Ď
MOTA	7240	CA	VAL 1					105.989				31.44	D
ATOM	7241	CB	VAL I					105.679				30.80	D
ATOM	7242		VAL I					106.540				23.78	D
ATOM	7243		VAL I					105.971				28.59	Ď
ATOM	7244	C	VAL 1					105.244			•	31.51	D
MOTA	7245	ō	VAL I					104.021				30.40	D
ATOM	7246	N	THR					105.990				32.62	D
ATOM	7247	CA	THR I					105.405					D
ATOM	7248	CB	THR					105.930				35.93	. D
ATOM	7249		THR I					105.430				37.09	D
ATOM	7250	CG2						105.488				34.89	D
ATOM	7251	C	THR I					105.679				32.81	D
ATOM	7252	ŏ	THR I					106.814				35.99	
ATOM	7252	И	PHE					104.628					D
ATOM	7254	CA	PHE				-	104.628				30.23	D
ATOM	7255	CB										29.91	D
ATOM	7256		PHE I					103.634				29.19	D
ATOM		CG	PHE 1					103.834				31.68	D
ATOM	7257		PHE I					103.451				29.72	D
MOTA	7258		PHE I					104.475				35.46	D
ATOM	7259	CRI	PHE I	U 2'	/0	\$0.5T	.9	103.704	19/	. /04	T.00	34.64	D

						•					
ATOM	7260	CE2	PHE	Ď	276	79.997	104.737	195.648	1.00	32.43	D
MOTA	7261	CZ			276	80.939	104.350	196.593	1.00	31.28	. р
ATOM	7262	C		-	276	74.607	104.656	198.111	1.00	28.75	ם
MOTA	7263	0			276	74.021	103.683	198.568		28.84	D
MOTA	7264	N			277	73.970	105.678	197.557	1.00	28.81	D
MOTA	7265	CA	VAL	D	277	72.521	105.683	197.465	1.00	31.28	D
MOTA	7266	CB	VAL	D	277	71.952	107.063	197.763	1.00	33.59	D
MOTA	7267	CG1	VAL	D	277	70.446	106.970	197.865	1.00	29.66	D
MOTA	7268	CG2			277			199.056	1.00	31.85	D
MOTA	7269	C	VAL	D	277	72.031	105.262	196.094	1.00	30.61	D
MOTA	7270	0			277			195.088		30.84	D
ATOM	7271	N			278			196.074	1.00	28.20	D
MOTA	7272	CA		_	278			194.836	1.00	25.49	D
MOTA	7273	CB			278			194.941	1.00	24.29	D
ATOM	7274	CG			278			195.008	1.00	23.28	D
MOTA	7275		TYR					196.164	_	14.76	D
ATOM	7276	CE1			278			196.224		25.52	a
ATOM	7277	CD2			278		100.778			14.90	D
ATOM	7278	CE2			278		100.114			25.25	D
MOTA	7279	CZ			278		100.158			26.04	D
ATOM	7280	OH			278	75.404		195.219		29.19	D.
MOTA	7281	C			278		104.329			26.91	D
ATOM	7282	0			278		104.474			26.77	D
ATOM	7283	N			279		104.678			27.38	D
ATOM	7284	CA			279		105.254			30.20	D
MOTA	7285	CB			279 279		106.005			24.11	D
ATOM .	7286	CD		-			106.689			32.89	, D
ATOM ATOM	728 7 7288	OE1			279 279		107.256			39.19	D
ATOM	7289	NE2			279		108.117 106.765			40.33	D
ATOM	7290	C			279		104.198			31.57	D
MOTA	7291	0			279		104.198			32.03	D
ATOM	7292	-	GLN				103.081			26.20	D D
ATOM	7293	C	GLY		1	55.769		90.619		46.04	E
MOTA	7294	ŏ	GLY		ī	55.952		90.252		50.74	E
ATOM	7295	N	GLY		ī	53.461		91.215		45.11	E
MOTA	7296	CA	GLY		1	54.504		90.220		46.37	E
MOTA	7297	N	VAL		2	56.623		91.400		39.60	E
ATOM	7298	CA	VAL		2	57.867		91.829		34.00	E
MOTA	7299	CB	VAL		2	58.076		93.343		31.98	Ē
ATOM	7300	CG1	VAL		2	59.460		93.709		31.97	E
MOTA	7301	CG2	VAL	E	2	57.027		94.107		26.73	E
MOTA	7302	С	VAL	E	2	59.020	43.942	91.071		35.29	E
MOTA	7303	0	VAL	E	2	59.137	42.717	91.031	1.00	36.08	E
ATOM	7304	N	ALA	Е	3	59.867	44.768	90.456	1.00	37.12	E
MOTA	7305	CA	ALA	Е	3	60.986	44.245	89.676	1.00	36.47	E
MOTA	7306	CB	ALA	Е	3	60.682	44.369	88.196	1.00	31.95	E
ATOM	7307	C	ALA	E	3	62.341	44.858	89.967	1.00	32.99	E
MOTA	7308	0	ALA		3	62.452	46.044	90.240	1.00	35.07	E
ATOM	7309	N	LEU		4	63.371	44.022	89.914	1.00	30.17	E
ATOM	7310	CA	LEU		4	64.722		90.140	1.00	28.06	E
MOTA	7311	CB	LEU		4	65.619		90.549		28.97	E
MOTA	7312	CG	LEU		4	65.232		91.821		27.63	E
MOTA	7313		LEU		4	66.355		92.198		26.09	E
MOTA	7314		LEU		4	64.965		92.922		26.55	E
ATOM	7315	C	LEU		4	65.223		88.834		31.45	E
ATOM	7316	0	LEU		4	64.792		87.751		33.65	E
ATOM	7317	N	GLY	E	5	66.138	46.028	88.940	1.00	31.71	E

MOTA	7318	CA	GLY	E	5	66.703	46.684	87.769	1.00 25.92	E
MOTA	7319	C	GLY	E	5	67.869	45.965	87.127	1.00 29.26	E
MOTA	7320	0	GLY	E	5	68.437	46.468	86.172	1.00 37.48	E
MOTA	7321	N	ALA	E	6	68.243	44.799	87.642	1.00 29.73	E
ATOM	7322	CA	ALA	E	6	69.341	44.019	87.066	1.00 30.56	E
MOTA	7323	CB	ALA	E	6	70.645	44.382	87.727	1.00 26.38	E
MOTA	7324	C	ALA	E	6	69.054	42.542	87.290	1.00 30.19	E
MOTA	7325	0	ALA	E	6	68.268	42.193	88.166	1.00 37.51	E
MOTA	7326	N	THR	E	7	69.685	41.676	86.516	1.00 22.98	E
ATOM	7327	CA	THR	E	7	69.474	40.255	86.681	1.00 21.43	E
ATOM	7328	CB	THR	E	7	69.254	39.549	85.328	1.00 20.53	E
ATOM	7329	OG1	THR	E	7	70.477	39.552	84.564	1.00 9.76	E
MOTA	7330	CG2	THR	E	7	68.115	40.242	84.554	1.00 15.59	E
MOTA	7331	C	THR	Е	7	70.680	39.646	87.362	1.00 26.69	E
MOTA	7332	0	THR	Е	7	70.826	38.424	87.416	1.00 28.87	. E
ATOM	7333	N	ARG	E	8	71.553	40.510	87.869	1.00 28.25	E
ATOM	7334	CA	ARG	E	8	72.763	40.085	88.575	1.00 26.99	E
MOTA	7335	CB	ARG	Е	8	73.712	39.314	87.670	1.00 24.88	E
MOTA	7336	CG	ARG	E	- 8	74.538	40.195	86.746	1.00 26.80	E
ATOM	7337	CD	ARG	E	8	74.293	39.869	85.288	1.00 27.21	E
MOTA	7338	NE	ARG	B	8	74.601	38.471	84.976	1.00 26.77	B
MOTA	7339	\mathbf{cz}	ARG	E	8	73.680	37.536	84.766	1.00 24.81	E
MOTA	7340	NHI	ARG	E	8	74.049	36.293	84.492	1.00 25.63	E
MOTA	7341	NH2	ARG	E	8	72.392	37.849	84.817	1.00 16.62	E
MOTA	7342	C	ARG	E	8	73.485	41.324	89.088	1.00 29.87	E
MOTA	7343	0	ARG	E	8	73.184	42.455	88.702	1.00 30.03	E
MOTA	7344	N	VAL	E	9	74.446	41.101	89.966	1.00 29.93	E
MOTA	7345	CA	VAL	E	9	75.184	42.188	90.555	1.00 27.67	E
MOTA	7346	CB	VAL	E	9	74.623	42.528	91.925	1.00 22.00	E
ATOM ·	7347	CG1	VAL	E	9	75.524	43.482	92.628	1.00 29.04	E
MOTA	7348	CG2	VAL	E	9	73.262	43.132	91.772	1.00 24.03	E
MOTA	7349	C	VAL	E	9	76.633	41.783	90.696	1.00 30.88	E
MOTA	7350	0	VAL	Ε	9	76.950	40.651	91.074	1.00 29.33	E
MOTA	7351	N	ILE	Ε	10	77.509	42.716	90.350	1.00 30.84	E
ATOM	7352	CA	ILE	E	10	78.929	42.495	90.461	1.00 31.61	E
MOTA	7353	CB	ILE	Ε	10	79.659	42.901	89.193	1.00 28.55	E
ATOM	7354	CG2	ILE	Е	10	81.153	42.678	89.361	1.00 27.36	E
MOTA	7355	CG1			10 -	79.160	42.044	88.038	1.00 26.74	E
ATOM	7356	CD1	ILE	E	10	79.449	40.568	88.194	1.00 25.91	E
MOTA	7357	C	ILE	E	10	79.404	43.353	91.600	1.00 33.90	E
MOTA	7358	0	ILE		10	79.274	44.570	⁹ 1.560	1.00 33.77	E
MOTA	7359	N	TYR		11	79.923	42.714	92.637	1.00 36.13	E
MOTA	7360	CA	TYR		11	80.417	43.458	93.781	1.00 37.06	E
MOTA	7361	CB	TYR		11	80.042	42.771	95.084	1.00 34.71	E
MOTA	7362	CG	TYR		11	80.051	43.713	96.257	1.00 39.58	E
MOTA	7363	CD1	TYR		11	78.883	44.356	96.659	1.00 41.57	E
MOTA	7364		TYR		11	78.879	45.263	97.711	1.00 38.13	E
ATOM	7365	CD2	TYR		11	81.226	44.001	96.943	1.00 37.32	E
ATOM	7366		TYR		11	81.230	44.915	98.000	1.00 38.53	E
MOTA	7367	CZ	TYR		11	80.049	45.542	98.375	1.00 36.39	E
ATOM	7368	OH	TYR		11	80.027	46.461	99.400	1.00 36.19	E
MOTA	7369	C	TYR		11	81.929	43.513	93.671	1.00 35.65	E
MOTA	7370	0	TYR		11	82.597	42.501	93.845	1.00 31.63	E
MOTA	7371	N	PRO		12	82.484	44.700	93.358	1.00 39.24	E
ATOM	7372	CD	PRO		12	81.743	45.915	92.978	1.00 41.90	E
ATOM	7373	CA	PRO		12	83.930	44.919	93.218	1.00 37.68	E
MOTA	7374	CB	PRO		12	84.019	46.312	92.605	1.00 35.89	E
ATOM	7375	CG	PRO	E	12	82.662	46.525	91.973	1.00 37.15	E

ATOM	7376	C	PRO	E	1.2	84.574	44.889	94.586	1.00 37.82		E
ATOM	7377	0	PRO	E	12	84.223	45.699	95.448	1.00 35.40		E
ATOM	7378	N	ALA		13	85.499	43.958	94.801	1.00 40.96		E
ATOM	7379	CA	ALA		13	86.162	43.877	96.093	1.00 45.60		E
ATOM	7380	CB	ALA		13	87.251	42.830	96.056	1.00 49.79		E
ATOM	7381	C	ALA		13	86.744	45.248	96.439	1.00 49.32		E
ATOM	7382	ō	ALA		13	87.463	45.853	95.639	1.00 50.92		E
ATOM	7383	Ŋ	GLY			86.407	45.745	97.625	1.00 50.32		E
					14						
ATOM	7384	CA	GLY		14	86.901	47.041	98.038	1.00 51.83		E
ATOM	7385	C	GLY		14	85.792	48.065	98.146	1.00 55.57		E
MOTA	7386	0	GLY		14	85.746	48.817	99.118	1.00 56.03		E
ATOM	7387	N	GLN		15	84.903	48.101	97.154	1.00 57.81		E
MOTA	7388	CA	GLN		15	83.793	49.050	97.150	1.00 58.83		E
MOTA	7389	CB	GLN		15	82.776	48.685	96.067	1.00 62.35		E
ATOM	7390	CG	GLN		15	83.354	48.547	94.670	1.00 68.58		E
ATOM	7391	CD	GLN		15 ·	83.252	49.815	93.843	1.00 71.63		E
MOTA	7392	OEI	GLN	E	15	83.691	50.887	94.262	1.00 74.06		E
ATOM	7393	NE2	GLN	E	15	82.673	49.695	92.651	1.00 74.53		E
ATOM	7394	С	GLN	E	15	83.107	49.024	98.504	1.00 60.94		E
MOTA	7395	0	GLN	E	15	82.876	47.963	99.077	1.00 61.51		B
ATOM	7396	N	LYS	E	16	82.784	50.193	99.027	1.00 63.19		E
ATOM	7397	CA	LYS	E	16	82.121	50.245	100.312	1.00 66.63		E
MOTA	7398	CB	LYS		16	82.074	51.681	100.822	1.00 73.67		E
ATOM	7399	CG	LYS		16	81.574	51.819	102.254	1.00 80.94		E
ATOM	7400	CD	LYS		16	81.362		102.642	1.00 87.89		E
MOTA	7401	CE	LYS		16	82.528		102.190	1.00 90.92		E
ATOM	7402	NZ	LYS		16	83.861		102.676	1.00 94.46		Ē
ATOM	7403	C	LYS		16	80.703		100.152	1.00 67.02		E
MOTA	7404	ō	LYS		16	80.126		101.092	1.00 70.07		E
ATOM	7405	N	GLN		17	80.147	49.869	98.952	1.00 64.08		E
MOTA	7406	CA	GLN		17	78.781	49.426	98.692	1.00 60.31		E
MOTA	7407	CB	GLN		17	77.808	50.268	99.514	1.00 59.69		E
ATOM			GLN		17	77.955	51.732	99.224			
	7408	CG	GLN						1.00 61.22 1.00 65.20		E
ATOM	7409	CD			17	76.698	52.513	99.493			E
ATOM	7410	OE1	GLN		17	76.180		100.622	1.00 64.50		E
ATOM	7411	NE2			17	76.194	53.197	98.453	1.00 58.46		E
ATOM	7412	C	GLN		17	78.361	49.517	97.226	1.00 54.80		E
MOTA	7413	0	GLN		17	78.794	50.403	96.502	1.00 57.05		E
MOTA	7414	N	VAL		18	77.504	48.595	96.802	1.00 48.39		E
ATOM	7415	CA	VAL		18	76.998	48.593	95.444	1.00 44.30		E
MOTA	7416	CB	VAL		18	77.286	47.278	94.738	1.00 44.09		E
ATOM	7417		VAL		18	76.675	47.290	93.351	1.00 43.03		E
ATOM	7418		VAL		18	78.780	47.072	94.641	1.00 49.03		E
ATOM	7419	C	VAL		18	75.499	48.782	95.560	1.00 45.32		\mathbf{E}
ATOM	7420	0	VAL		18	74.898	48.408	96.563	1.00 48.67		E
MOTA	7421	N	GLN		19	74.886	49.376	94.550	1.00 42.05		E
MOTA	7422	CA	GLN		19	73.465	49.596	94.625	1.00 41.76		E
MOTA	7423	CB	GLN		19	73.185	51.083	94.727	1.00 44.42		E
MOTA	7424	CG	GLN	E	19	73.948	51.916	93.749	1.00 53.82		E
MOTA	7425	CD	GLN	E	19	74.034	53.358	94.192	1.00 56.57		E
ATOM	7426	OE1	GLN	E	19	74.652	53.665	95.209	1.00 59.10	•	E
ATOM	7427		GLN		19	73.404	54.253	93.437	1.00 62.38		E
MOTA	7428	C	GLN		19	72.681	48.966	93.491	1.00 39.95		E
ATOM	7429	0	GLN		19	73.177	48.829	92.385	1.00 38.80		E
ATOM	7430	N	LEU		20	71.455	48.563	93.812	1.00 36.92		E
ATOM	7431	CA	LEU		20	70.542	47.910	92.891	1.00 30.32		E
MOTA	7432	CB	LEU		20	70.337	46.457	93.336	1.00 33.96		Ē
ATOM	7433	CG	LEU		20	69.434	45.520	92.521	1.00 37.59		E
	·										_

MOTA	7434	CD1	LEU	E 20	70.071	45.233	91.176	1.00 30.23	E
MOTA	7435	CD2	LEU	E 20	69.227	44.219	93.278	1.00 34.96	E
MOTA	7436	C	LEU	E 20	69.208	48.668	92.912	1.00 35.04	E
MOTA	7437	0	LEU	E 20	68.804	49.205	93.942	1.00 34.98	E
ATOM	7438	N	ALA	E 21	68.525	48.708	91.776	1.00 34.62	E
ATOM	7439	CA	ALA			49.424	91.692	1.00 32.72	E
ATOM	7440	CB	ALA			50.184	90.375	1.00 28.04	B
MOTA	7441	C	ALA			48.487	91.804	1.00 34.50	B
ATOM	7442	ō	ALA			47.342	91.351	1.00 33.01	E
ATOM	7443	N	VAL			48.997	92.410	1.00 36.31	E
ATOM	7444	CA	VAL			48.249	92.580	1.00 38.07	E
ATOM	7445	CB	VAL			47.893	94.036	1.00 39.99	E
MOTA	7446		VAL			46.594	94.085	1.00 34.81	E
ATOM	7447		VAL			47.819	94.829	1.00 40.01	E
ATOM	7448	C	VAL			49.207	92.176	1.00 41.59	E
ATOM	7449	ō	VAL			50.384	92.552	1.00 42.62	E
ATOM	7450	N	THR			48.690	91.436	1.00 43.32	E
ATOM	7451	CA	THR			49.502	90.988	1.00 45.01	E
ATOM	7452	CB	THR			49.923	89.539	1.00 46.09	E
ATOM	7453		THR			50.362	88.967	1.00 56.87	E
MOTA	7454	CG2				48.769	88.737	1.00 51.13	E
MOTA	7455	C	THR			48.696	91.134	1.00 44.67	E
ATOM	7456	Õ	THR			47.503	90.852	1.00 41.77	E
ATOM	7457	N	ASN			49.369	91.603	1.00 47.65	E
ATOM	7458	CA	ASN :			48.782	91.820	1.00 47.63	E
MOTA	7459	CB	ASN :			49.126	93.232	1.00 44.81	E
ATOM	7460	CG	ASN :			48.716	93.484		E
			ASN .			47.823		1.00 48.83	
ATOM	7461 7462		ASN :			49.357	92.820 94.462	1.00 48.83	E.
ATOM ATOM	7462	C	ASN :			49.334	90.786	1.00 47.77	E
ATOM	7464	Q N	ASN :			50.526		1.00 51.24	E
ATOM	7465	N				48.452	89.895	1.00 54.60	E
ATOM	7466	CA	ASN :			48.783	88.811	1.00 58.05	E
MOTA	7467	CB	ASN :			47.628	87.815	1.00 55.36	E
ATOM	7468	CG	ASN :			47.372	87.106	1.00 55.70	E
ATOM	7469		ASN :			47.607	87.650	1.00 53.11	E
ATOM	7470		ASN :			46.862	85.887	1.00 59.68	E
ATOM	7471	C	ASN :			49.069	89.285	1.00 61.01	E
ATOM	7472	0	ASN :			50.110	88.985	1.00 64.11	E
ATOM	7473	N	ASP :			48.111	90.006	1.00 61.50	E
MOTA	7474	CA	ASP :			48.216	90.508	1.00 63.45	E
ATOM	7475	CB	ASP :			47.189	91.603	1.00 67.89	E
MOTA	7476	CG	ASP			45.776	91.098	1.00 67.98	E
ATOM	7477		ASP			44.850	91.929	1.00 67.86	E
ATOM	7478		ASP			45.598	89.875	1.00 68.04	E
MOTA	7479	C	ASP				. 91.007		Ē
ATOM	7480	0	ASP			49.947	92.150	1.00 62.99	E
ATOM	7481	N	GLU			50.325	90.128	1.00 67.19	E
ATOM	7482	CA	GLU			51.668	90.422	1.00 70.83	E
MOTA	7483	CB	GLU :			52.136	89.300	1.00 75.40	E
ATOM	7484	CG	GLU			52.567	88.037	1.00 88.94	E
ATOM	7485	CD	GLU			52.306	86.733	1.00 93.88	E
MOTA	7486		GLU			52.720	86.620	1.00 99.08	Ε
MOTA	7487		GLU			51.695	85.818	1.00 94.17	E
MOTA	7488	C	GLU :			51.788	91.771	1.00 69.46	E
MOTA	7489	0	GLU			52.875	92.331	1.00 68.88	E
MOTA	7490	N	ASN			50.684	92.310	1.00 69.07	E
MOTA	7491	CA	ASN	E 28	47.959	50.770	93.591	1.00 71.81	E

ATOM	7492	CB	ASN	E	28	46.517	51.256	93.381	1.00 77.	74 E
ATOM	7493	CG	ASN	E	28	45.772	50.452	92.323	1.00 80.	
ATOM	7494		ASN		28	44.694	50.850		1.00 79.	
	7495		ASN			46.343				
ATOM					28		49.317		1.00 81.	
MOTA	7496	C	ASN		28	47.976	49.487		1.00 71.	
ATOM	7497	0	ASN	E	28	47.183	48.582	94.175	1.00 74.	
MOTA	7498	N	SER	E	29	48.889	49.441	95.357	1.00 70.	27 E
ATOM	7499	CA	SER	E	29	49.085	48.302	96.244	1.00 68.	
ATOM	7500	CB	SER		29	49.056	46.983	95.460	1.00 70.	
ATOM	7501	OG	SER		29	50.068	46.950	94.465	1.00 72.	
ATOM	7502	C	SER							
					29	50.461	48.501	96.872	1.00 64.	
ATOM	7503	0	SER		29	51.471	48.521	96.173	1.00 65.	
MOTA	7504	N	THR		30	50.503	48.668	98.185	1.00 60.	BO E
MOTA	7505	CA	THR	E	30	51.776	48.878	98.848	1.00 58.	83 E
MOTA	7506	CB	THR	E	30	51.577	49.543	100.215	1.00 59.0	00 E
MOTA	7507	OG1	THR	E	30	50.777	50.721	100.060	1.00 63.0	
MOTA	7508	CG2	THR	E	30	52.902		100.794	1.00 64.3	
ATOM	7509	C	THR		30	52.502	47.554	99.027	1.00 54.3	
ATOM	7510		THR		30					- -
		0				51.896	46.491	98.950	1.00 56.3	_
MOTA	7511	N	TYR		31	53.808	47.625	99.242	1.00 50.3	
MOTA	7512	CA	TYR		31	54.620	46.431	99.447	1.00 48.4	42 E
MOTA	7513	CB	TYR	E	31	55.301	46.004	98.158	1.00 46.2	28 E
ATOM	7514	CG	TYR	E	31	54.409	45.324	97.168	1.00 48.1	73 E
MOTA	7515	CD1	TYR	E	31	54.081	45.936	95.957	1.00 48.2	
ATOM	7516	CE1	TYR	E	31	53.325	45.269	95.007	1.00 52.8	
MOTA	7517		TYR		31	53.950	44.033	97.401	1.00 51.2	_
ATOM	7518	CE2	TYR		31	53.194	43.354			
								96.452	1.00 51.1	
ATOM	7519	CZ	TYR		31	52.888	43.975	95.261	1.00 53.1	
ATOM	7520	OH	TYR		31	52.169	43.287	94.316	1.00 60.8	36 E
MOTA	7521	C	TYR	E	31	55.714	46.675	100.474	1.00 47.2	23 E
MOTA	7522	0	TYR	Ε	31	56.178	47.799	100.673	1.00 48.9	94 E
MOTA	7523	N	LEU	E	32	56.116	45.609	101.141	1.00 43.2	
ATOM	7524	CA	LEU	E	32	57.188	45,698	102.103	1.00 41.0	
ATOM	7525	CB	LEU		32	56.831		103.394	1.00 48.0	
ATOM	7526	CG	LEU	_	32	56.084		104.452	1.00 48.2	
ATOM	7527		LEU		32	55.647		105.573		
									1.00 51.4	
MOTA	7528		PEA		32	56.985		104.969	1.00 45.4	_
ATOM	7529	C	LEU		32	58.332		101.414	1.00 41.9	
MOTA	7530	0	LEU		32	58.222	43.812	101.025	1.00 37.7	70 B
ATOM	7531	N	ILE	E	33	59.420	45.715	101.229	1.00 37.6	51 E
ATOM	7532	CA	ILE	E	33	60.576	45.146	100.590	1.00 34.9	91. E
ATOM -	7533	CB	ILE	E	33	61.274	46.201	99.735	1.00 36.7	77 E
MOTA	7534	CG2	ILE	Е	33	62.455	45.589	98.986	1.00 35.3	
ATOM	7535		ILE		33	60.248	46.828	98.786	1.00 35.9	
ATOM	7536		ILE		33	59.432	45.825	97.997	1.00 27.3	
ATOM	7537	C	ILE							
					33	61.506		101.677	1.00 36.0	
MOTA	7538	0	ILE		33	61.890		102.580	1.00 37.1	
MOTA	7539	N	GLN		34	61.848		101.590	1.00 36.5	
ATOM	7540	CA	GLN	E	34	62.736		102.553	1.00 38.1	L3 E
MOTA	7541	CB	GLN	E	34	61.952	41.723	103.364	1.00 42.9	99 E
MOTA	7542	CG	GLN	E	34	62.462		104.751	1.00 43.0	
MOTA	7543	CD	GLN		34	61.560		105.516	1.00 45.8	_
ATOM	7544		GLN		34	61.405		105.157	1.00 50.9	
ATOM	7545		GLN		34					
						60.943		106.571	1.00 45.0	
ATOM	7546	C	GLN		34	63.806		101.722	1.00 36.6	
MOTA	7547	0	GLN		34	63.508		100.971	1.00 35.1	
MOTA	7548	N	SER		35	65.050	42.483	101.862	1.00 36.6	
MOTA	7549	CA	SER	E	35 ⁻	66.138	41.910	101.083	1.00 37.2	23 E
•										

ATOM	7550	CB	SER I	3 3!	5	66.759	43.006	100.221	1.00	40.58	E
ATOM	7551	OG	SER			65.744	43.789	99.628		52.81	E
MOTA	7552	C	SER I			67.231		101.919		34.80	E
ATOM	7553	ō	SER I			67.469		103.055		40.19	E
ATOM	7554	N	TRP I			67.899		101.347			
MOTA	7555 7555	CA	TRP							29.82	E
						69.004		102.026		30.01	E
ATOM	7556	CB	TRP I			68.500		103.074		19.84	E
ATOM	755 7	CG	TRP 1			67.917.		102.516	1.00	24.65	E
MOTA	7558	CD2				66.571	37.200	102.068	1.00	21.26	E
MOTA	7559	CE2	TRP 1		5	66.466	35.871	101.597	1.00	26.04	E
ATOM	7560	CE3	TRP I	3 36	5	65.443	38.026	102.024	1.00	19.55	E
MOTA	7561	CD1	TRP I	3 3 6	5	68.560	36.199	102.306	1.00	25.27	E
ATOM	7562	NE1	TRP I	3 -36	5	67.695		101.753		27.64	E
ATOM	7563	CZ2	TRP I	3 36	5	65.269		101.084		21.61	Ē
ATOM	7564	CZ3	TRP I			64.243		101.517		18.87	E
ATOM	7565	CH2	TRP I			64.170		101.055		21.25	E
ATOM	7566	C	TRP I			69.891		101.017			
ATOM	7567	ō	TRP I							29.36	E
						69.573	38.787	99.833		29.46	E
ATOM	7568	N	VAL I			71.009		101.495		27.63	E
MOTA	7569	CA	VAL I			71.923		100.622		28.21	E
ATOM	7570	CB	VAL I			73.158	38.574	100.344	1.00	29.01	E
ATOM	7571		VAL I			74.122	37.842	99.439	1.00	30.04	E
MOTA	7572		VAL I			72.724	39.869	99.707	1.00	25.95	E
MOTA	7573	C	VAL I	37	7	72.362	36.409	101.267	1.00	28.25	E
ATOM	7574	0	VAL I	37	7	72.847	36.405	102.393	1.00	33.23	E
ATOM	7575	N	GLU F	38	3	72.178	35.315	100.547		26.36	· E
ATOM	7576	CA	GLU E	38	3	72.584	34.011	101.031		28.53	E
ATOM	7577	CB	GLU E	38	3	71.531		100.670		24.91	· E
ATOM	7578	CG	GLU I			70.183		101.281		33.69	. E
ATOM	7579	CD	GLU I			69.091		100.729		33.38	
ATOM	7580		GLU I			69.453		100.729			
ATOM	7581		GLU H			67.894				31.38	E
ATOM								100.867		28.30	E
	7582	C	GLU E			73.884		100.328		30.16	E
ATOM	7583	0	GLU E			74.184	34.307	99.295		32.61	E
ATOM	7584	N	ASN E			74.679		100.895		30.97	E
ATOM	7585	CA	ASN E			75.930		100.254		30.12	E
MOTA	7586	CB	ASN' E			76.990	32.038	101.273	1.00	30.70	E
ATOM	7587	CG	ASN E			76.626	30.768	102.021	1.00	39.43	Е
ATOM	7588		ASN E		•	75.807	29.965	101.566	1.00	42.90	E
MOTA	7589	ND2	ASN E	39	•	77.253	30.571	103.171	1.00	40.16	E
MOTA	7590	C	ASN E	39	•	75.642	31.315	99.291	1.00	30.88	E
ATOM	7591	0	ASN E	39	•	74.488	30.902	99.138	1.00	24.86	E
MOTA	7592	N	ALA E	40)	76.695	30.811	98.651		32.96	E
ATOM	7593	CA	ALA E	40)	76.569	29.745	97.674		33.48	E
ATOM	7594	CB	ALA E			77.923	29.317	97.220		35.60	Ē
MOTA	7595	C	ALA E			75.794	28.552	98.193		37.35	E
ATOM	7596	ō	ALA E			75.035	27.939	97.458		38.58	_
ATOM	7597	N	ASP E								E
						75.974	28.212	99.459		39.62	E
ATOM	7598	CA	ASP E			75.258	27.076	99.995		43.38	E.
MOTA	7599	CB	ASP E			75.998		101.191		47.76	E
ATOM .	7600	CG	ASP E			77.280		100.792		50.10	E
ATOM	7601		ASP E			77,233	24.996	99.856		50.92	E
ATOM	7602		ASP E			78.325		101.416		50.93	E
MOTA	7603	C	ASP E		L	73.818	27.373	100.369	1.00	45.89	E
MOTA	7604	0	ASP E	41		73.110	26.496	100.849	1.00	51.61	E
MOTA	7605	N	GLY E	42	?	73.379		100.146		43.17	E
MOTA	7606	CA	GLY E			72.008 .		100.461	-	37.95	E
ATOM	7607	C	GLY E			71.805		101.886		37.65	Ē
											_

ATOM	7608	0	GLY	T /	2	70.680	20 692	102.277	1 00	38.17	כז
ATOM	7609	N									E
			VAL		.3	72.869		102.678		38.96	E
ATOM	7610	CA	VAL		3	72.687		104.055		39.36	E
MOTA	7611	CB	VAL		.3	73.606	29.134	105.041	1.00	34.67	E
ATOM	7612	CG1	VAL	E 4	3	74.302	28.008	104.334	1.00	32.49	E
ATOM	7613	CG2	VAL	E 4	3	74.590	30.061	105.701	1.00	39.40	E
ATOM	7614	C	VAL	E 4	3	72.874		104.229		41.65	E
ATOM	7615	0	VAL		3	73.755		103.611		41.79	E
ATOM	7616	N	LYS		4	72.022		105.068			
ATOM	7617	CA	LYS							40.31	E
					4	72.069		105.333		41.11	E
ATOM	7618	CB	LYS		4	70.749		105.945		41.89	E
ATOM	7619	CG	LYS		4	69.497		105.101		41.17	E
ATOM	7620	CD	LYS		4	68.484	32.872	105.826	1.00	45.18	E
ATOM	7621	CE	LYS :	E 4	4	67.213	32.708	105.026	1.00	47.59	E
ATOM	7622	NZ	LYS :	E 4	4	66.586	34.029	104.799	1.00	55.78	E
MOTA	7623	C	LYS :	E 4	4	73.195		106.300		43.34	Ē
ATOM	7624	0	LYS		4	72.955		107.498		41.72	E
ATOM	7625	N	ASP :			74.429		105.814			
ATOM	7626									44.22	E
		CA	ASP :			75.496		106.703		43.51	E
ATOM	7627	CB	ASP :			76.854		106.261		46.06	E
ATOM	7628	CG	ASP :			77.064	33.884	104.780	1.00	45.99	E
ATOM	7629	OD1	ASP I			76.505	34.822	104.171	1.00	48.45	E
MOTA	7630	OD2	ASP :	B 4	5	77.805	33.041	104.239	1.00	35.15	E
ATOM	7631	C	ASP :	Ė 4	5	75.418	35.778	106.547		45.51	E
MOTA	7632	0	ASP 1	E 4	5	74.549		105.825		50.35	E
MOTA	7633	N	GLY :			76.308		107.183		45.87	E
ATOM	7634	CA	GLY I			76.179		107.065		45.12	E
ATOM	7635	C	GLY I			77.190		106.152			
ATOM										45.17	E
	7636	0	GLY I			77.455		106,259		46.18	E
ATOM	7637	N	ARG I			77.754		105.256		43.73	E
ATOM	7638	CA	ARG 1			78.761		104.338	1.00	40.06	E
ATOM	7639	CB	ARG 1	E 4	7	79.084	37.202	103.300	1.00	47.98	E
MOTA	7640	CG	ARG :	E 4	7	80.439	36.575	103.522	1.00	58.67	E
MOTA	7641	CD	ARG I	E 4	7	80.465	35.732	104.771	1.00	67.69	E
MOTA	7642	NE	ARG I	E 4	7	81.817	35.259	105.047	1.00	78.50	E
ATOM	7643	CZ	ARG I	E 4	7	82.764	36.007	105.606		86.38	E
ATOM	7644	NH1	ARG I			82.498		105.954		90.89	E
ATOM	7645		ARG			83.978		105.816		91.15	E
ATOM	7646	C	ARG I			78.350		103.663			
										39.17	B
ATOM	7647	0	ARG I			79.172		103.450		38.55	E
ATOM		.N	PHE I			77.075		103.332		37.09	E
	7649	CA	PHE 1			76.606		102.694		38.80	E
ATOM	7650	CB	PHE I	E 4	8	76.395	40.685	101.181	1.00	36.91	E
MOTA	7651	CG	PHE 1	E 4	8	77.669	40.490	100.429	1.00	33.48	E
ATOM	7652	CD1	PHE 1	E 4	8	78.232	39.222	100.308	1.00	35.80	E
MOTA	7653	CD2	PHE :	E 4	8	78.369	41.591	99.935	1.00	35.12	E
ATOM	7654	CEL	PHE I	E 4	8	79.475	39.053	99.719		32.89	E
MOTA	7655		PHE			79.609	41.441	99.346		30.41	Ē
ATOM	7656	CZ	PHE			80.171	40.173	99.237		33.91	
	7657	C	PHE I			75.325					E
								103.340		35.91	E
	7658	0	PHE			74.501		103.721		33.62	E
	7659	N	ILE I			75.166		103.456		36.47	E
	7660	CA	ILE 1			73.978		104.061		38.80	E
	7661	CB	ILE :		9	74.329	43.872	105.415	1.00	43.00	E
MOTA	7662	CG2	ILE I	E 4	9	73.105	44.516	106.050	1.00	39.31	E
MOTA	7663		ILE I			74.827		106.333		46.46	E
,	7664		ILE 1			75.603		107.517		55.41	Ē
ATOM	7665	Ç	ILE :			73:350		103.132		36.76	E
		-		_ =	-				1.00		17

ATOM	7666	0	ILE E	49	74.036	45.066	102.503	1.00 39.2	0 E
MOTA	7667	N	VAL E	50	72.032	44.239	103.046	1.00 34.7	
MOTA	7668	CA	VAL E	50	71.317	45.134	102.160	1.00 37.9	3 E
ATOM	7669	CB	VAL E	50	70.330	44.341	101.261	1.00 39.5	
MOTA	7670	CG1	VAL E	50	69.669	45.266	100.257	1.00 36.6	
MOTA	7671		VAL E	50	71.061	43.201		1.00 38.2	
MOTA	7672	C	VAL E	50	70.528	46.127		1.00 38.9	
ATOM	7673	Ō	VAL E	50	69.997	45.778		1.00 41.6	
ATOM	7674	N	THR E	51	70.453	47.364		1.00 38.1	
ATOM	7675	CA	THR E	51	69.677	48.382		1.00 36.5	
ATOM	7676	CB	THR E	51	70.551	49.391		1.00 40.1	
ATOM	7677		THR E	51	71.482	49.996		1.00 47.1	
ATOM	7678	CG2	THR E	51	71.301	48.717		1.00 47.7	
ATOM	7679	C	THR E	51	68.887	49.175		1.00 34.8	_
ATOM	7680	ŏ	THR E	51	69.318	49.367		1.00 38.3	
ATOM	7681	N	PRO E	52	67.692	49.606		1.00 33.4	
ATOM	7682	CD	PRO E	52	67.019	50.775		1.00 34.5	_
ATOM	7683	CA	PRO E	52	67.163	49.313		1.00 34.0	
ATOM	7684	CB	PRO E	52	66.013	50.308		1.00 32.3	
ATOM	7685	CG	PRO E	52	65.688	50.716		1.00 38.5	
ATOM	7686	C	PRO E	52	66.690	47.873		1.00 34.9	
ATOM	7687	ō	PRO E	52	66.071	47.360		1.00 39.1	
ATOM	7688	N	PRO E	53	66.981	47.197		1.00 31.8	
MOTA	7689	CD	PRO E	53	67.614	47.687		1.00 30.3	
ATOM	7690	CA	PRO E	53	66.552	45.808		1.00 29.5	
ATOM	7691	CB	PRO E	53	67.074	45.431		1.00 30.6	
MOTA	7692	CG	PRO E	53	67.043	46.759		1.00 25.1	
ATOM	7693	C	PRO E	53	65.044	45.603		1.00 30.5	
ATOM	7694	0	PRO E	53	64.589	44.497		1.00 29.6	
ATOM	7695	N	LEU E	54	64.269	46.666		1.00 33.0	
ATOM .	7696	CA	LEU E	54	62.806	46.571		1.00 34.0	
MOTA	7697	CB	LEU E	54	62.259	46.017	106.564	1.00 34.2	
MOTA	7698	CG	LEU E	54	60.740	45.916	106.662	1.00 36.1	
MOTA	7699	CD1	LEU E	54	60.270	44.653	105.941	1.00 41.5	4 E
ATOM	7700	CD2	LEU E	54	60.336	45.866	108.124	1.00 35.9	5 E
MOTA	7701	С	LEU E	54	62.181	47.930	105.048	1.00 36.1	1 E
MOTA	7702	0	LEU E	54	62.406	48.836	105.855	1.00 41.1	3 E
ATOM	7703	N	PHE E	55	61.388	48.078	103.992	1.00 31.8	
MOTA	7704	CA	PHE E	55	60.758	49.365	103.709	1.00 34.5	5 E
MOTA	7705	CB	PHE E	55	61.755	50.322	103.057	1.00 34.7	4 E
MOTA	7706	CG	PHE E	55	. 62.247	49.857	101.725	1.00 41.5	2 E
MOTA	7707	CD1	PHE E	55	61.644	50.294	100.551	1.00 46.1	3 E
MOTA	7708	CD2	PHE E	55	63.296	48.950	101.641	1.00 43.2	3 E
ATOM	7709	CE1	PHE E	55	62.084	49.832	99.300	1.00 46.5	3 E
MOTA	7710	CE2	PHE E	55	63.740	48.485	100.407	1.00 49.5	9 E
MOTA	7711	CZ	PHE E	55	63.134	48.925	99.231	100 48.4	7 E
MOTA	7712	C	PHE E	55	59.565	49.205	102.801	1.00 37.8	0 E
MOTA	7713	0	PHE E	55	59.388	48.158	102.164	1.00 39.4	
MOTA	7714	N	ALA E	56	58.747	50.252	102.732	1.00 41.2	6 E
MOTA	7715	CA	ALA E	56	57.544	50.215	101.906	1.00 40.5	3 E
ATOM	7716	CB	ALA E	. 56	56.368	50.739	102.700	1.00 36.3	8 E
MOTA	7717	С	ALA E	56	57.640	50.957	100.574	1.00 39.6	1 E
MOTA	7718	0	ALA E	56	58.326	51.971	100.437	1.00 40.5	6 E
ATOM	7719	N	MET E	57	56.957	50.416	99.582	1.00 40.8	
MOTA	7720	CA	MET E	57	56.896	51:025	98.269	1.00 42.3	
MOTA	7721	CB	MET E	57	57.570	50.149	97.223	1.00 41.0	
ATOM	7722	CG	MET E	57	59.033	49.903	97.488	1.00 43.9	
MOTA	7723	SD	MET E	57	59.975	49.889	95.957	1.00 44.9	3 E

MOTA	7724	CE	MET I	E 57	59.317	48.456	95.232	1.00 52.13	E
MOTA	7725	C	MET 1	E 57	55.406	51.139	97.986	1.00 44.69	. E
MOTA	7726	0	MET I	5 57	54.722	50.134	97.758	1.00 43.13	E
ATOM	7727	N	LYS I	3 58	54.905	52.366	98.038	1.00 45.78	E
MOTA	7728	CA	LYS I	58	53.496	52.614	97.803	1.00 53.73	E
ATOM	7729	CB	LYS I	E 58	53.006	53.704	98.756	1.00 60.16	E
MOTA	7730	CG	LYS I	5 8	51.500	53.755	98.917	1.00 66.91	E
MOTA	7731	CD	LYS I	E 58	51.090	54.908	99.820	1.00 73.01	E
MOTA	7732	CE	LYS I	E 58	49.734	54.648	100.470	1.00 77.37	E
ATOM	7733	NZ	LYS I	E 58	49.784	53.487	101.417	1.00 74.60	E
· MOTA	7734	С	LYS F	S 58	53.222	53.022	96.355	1.00 54.93	É
ATOM	7735	0	LYS E	S 58	53.727	54.038	95.877	1.00 57.77	E
MOTA	7736	N	GLY F	3 59	52.415	52.225	95.662	1.00 54.84	E
MOTA	7737	CA	GLY F	3 59	52.087	52.532	94.283	1.00 52.96	E
ATOM	7738	С	GLY E	E 59	53.328	52.590	93.421	1.00 51.28	E
MOTA	7739	0	GLY I	5 5 9	54.401	52.216	93.877	1.00 46.55	E
MOTA	7740	N	LYS E	60	53.185	53.057	92.181	1.00 54.00	E
MOTA	7741	CA	LYS E	3 60	54.318	53.146	91.264	1.00 57.19	E
MOTA	7742	CB	LYS E	60	53.884	53.715	89.910	1.00 57.37	E
MOTA	7743	CG	LYS E	60	52.787	52.902	89.230	1.00 60.55	E
MOTA	7744	CD	LYS E	60	52.817	53.027	87.716	1.00 62.15	E
ATOM	7745	CE	LYS E	3 60	54.054	52.354	87.136	1.00 73.56	E
MOTA	7746	NZ	LYS E	60	54.071	52.347	85.637	1.00 79.09	E
MOTA	7747	С	LYS E	60	55.385	54.033	91.873	1.00 58.12	E
ATOM	7748	Ο.	LYS E	60	55.223	55.248	91.948	1.00 61.52	E.
ATOM	7749	N	LYS E	61	56.470	53.410	92.314	1.00 54.03	E
MOTA	7750	CA	LYS E	61	57.571	54.118	92.943	1.00 49.88	E
ATOM	7751	CB	LYS E	61	57.462	54.013	94.466	1.00 53.55	E
ATOM	7752	CG	LYS E	61	57.350	55.347	95.189	1.00 60.82	· E
MOTA	7753	CD	LYS E	61	58.333	55.426	96.352	1.00 66.40	E
ATOM	7754 ⁻	CE	LYS E	61	58.074	54.343	97.407	1.00 73.51	E
ATOM	7755	NZ	LYS E	61	59.112	54.322	98.500	1.00 73.88	E
MOTA	7756	C	LYS F	61	58.869	53.478	92.487	1.00 48.76	E
MOTA	7757	0	LYS E	61	58.865	52.448	91.813	1.00 47.59	E
ATOM	7758	N	GLU E	62	59.982	54.092	92.855	1.00 48.58	E
MOTA	7759	CA	GLU F	62	61.291	53.568	92.493	1.00 48.54	E
MOTA	7760	CB	GLU I	62	61.758	54.205	. 91.187	1.00 49.67	E
ATOM	7761	CG	GLU F	62	62.532	53.266	90.293	1.00 66.30	E
ATOM	7762	CD	GLU E	62	64.030	53.503	90.345	1.00 74.23	E
MOTA	7763	OE1	GLU E	62	64.594	53.523	91.464	1.00 81.46	E
ATOM	7764	OE2	GLU E	62	64.642	53.664	89.262	1.00 72.93	E
ATOM	7765	C	GLU E	62	62.231	53.911	93.640	1.00 43.78	E
MOTA	7766	0	GLU E	62	62.229	55.031	94.138	1.00 49.05	E
MOTA	7767	N	ASN E	63	63.002	52.944	94.103	1.00 39.78	E
MOTA	7768	CA	ASN I	63	63.921	53.223	95.196	1.00 39.94	E
MOTA	7769	CB	ASN I	63	63.374	52.781	96.550	1.00 41.74	E
MOTA	.7770	CG	ASN I		62.123	53.508	96.939	1.00 46.44	E
MOTA	7771	OD1	ASN I	3 63	61.023	53.093	96.594	1.00 52.81	E
MOTA	7772	ND2	ASN I	63	62.278	54.607	97.660	1.00 48.86	E
MOTA	7773	C	ASN I	63	65.185	52.475	94.947	1.00 38.50	E
MOTA	7774	0	ASN I	63	65.254	51.659	94.022	1.00 41.77	E
ATOM	7775	N	THR I	64	66.175	52.728	95.792	1.00 34.77	E
MOTA	7776	CA	THR I	S 64	67.457	52.074	95.635	1.00 35.48	E
MOTA	7777	CB	THR I	64	68.565	53.087	95.388	1.00 31.59	E
MOTA	7778	OG1	THR E	64	68.189	53.952	94.310	1.00 43.11	E
ATOM	7779	CG2			69.853	52.368	95.039	1.00 29.61	E
ATOM	7780	C	THR I		67.903	51.203	96.790	1.00 37.96	E
ATOM	7781	0	THR E	64	67.898	51.625	97.948	1.00 41.89	E

ATOM	7782	N	LEU E	65	68.298	49.982	96.456	1.00 38.28	E
ATOM	7783	CA	LEU E		68.805	49.049	97.438	1.00 39.90	E
ATOM	7784	CB	TEA H		68.403	47.627	97.072	1.00 34.15	E
ATOM	7785	CG	LEU H		66.913	47.328	97.194	1.00 33.31	E
ATOM	7786	CD1			66.655	45.867	96.904		
MOTA	7787	CD2	LEU I		66.446			1.00 32.75	E
-						47.670	98.590	1.00 39.57	E
ATOM	7788	C	LEU I		70.324	49.186	97.398	1.00 43.55	E
MOTA	7789	0	LEU I		70.895	49.323	96.316	1.00 42.02	E
ATOM	7790	N	ARG E		70.966	49.184	98.568	1.00 45.20	\mathbf{E}
ATOM	7791	CA	ARG E		72.419	49.298	98.646	1.00 46.33	E
MOTA	7792	CB	ARG E	66	.72.813	50.546	99.441	1.00 48.13	E
MOTA	7793	CG	ARG E	66	72.296	51.836	98.836	1.00 53.95	E
MOTA	7794	CD	ARG E	66	72.547	53.023	99.750	1.00 60.84	E
MOTA	7795	NE	ARG F	66	71.634	54.132	99.476	1.00 59.54	E
MOTA	7796	CZ	ARG E	66	71.674	54.880	98.383	1.00 58.20	E
MOTA	7797	NH1	ARG E	66	72.589	54.640	97.459	1.00 60.32	E
MOTA	7798	NH2	ARG E	66	70.792	55.859	98.213	1.00 59.58	E
MOTA	7799	C	ARG E		72.977	48.054	99.314	1.00 45.37	Ē
ATOM	7800	ō	ARG E		72.567		100.428	1.00 47.47	E
ATOM	7801	N	ILE E		73.898	47.378	98.627	1.00 40.37	E
ATOM	7802	CA	ILE E		74.505	46.161	99.149	1.00 41.48	E
MOTA	7803	CB	ILE E		74.751	45.113			
MOTA	7803	CG2	ILE E				98.040	1.00 39.97	E
					75.517	43.937	98.606	1.00 42.72	E
MOTA	7805	CG1	ILE E		73.427	44.615	97.461	1.00 41.26	·E
MOTA	7806	CD1	ILE E		72.791	45.560	96.487	1.00 40.50	E
MOTA	7807	C	ILE E		75.839	46.456	99.825	1.00 44.21	E
ATOM	7808	0	ILE E		76.792	46.931	99.196	1.00 42.82	E
	7809	N	LEU E		75.911		101.110	1.00 42.88	E
MOTA	7810	CA	LEU E	68	77.117	46.398	101.865	1.00 42.67	E
MOTA	7811	CB	LEU E	68	76.766	47.039	103.196	1.00 43.76	E
MOTA	7812	CG	LEU E	68	75.778	48.187	103.174	1.00 38.58	E
MOTA	7813	CD1	LEU E	68	75.549	48.617	104.596	1.00 38.98	E
MOTA	7814	CD2	LEU E	68	76.315	49.325	102.342	1.00 43.96	. E
MOTA	7815	С	LEU E	68	77.954		102.126	1.00 44.23	E
MOTA	7816	0	LEU E	68	77.442	44.098	102.493	1.00 40.01	E
MOTA	7817	N	ASP E	69	79.260		101.953	1.00 46.40	E
ATOM	7818	CA	ASP E		80.246	44.301		1.00 46.31	E
MOTA	7819	CB	ASP E		81.518		101.430	1.00 45.34	E
ATOM	7820	ĊG	ASP E		82.667		101.650	1.00 51.39	Ē
MOTA	7821		ASP E		83.730		101.031	1.00 54.71	E
ATOM	7822		ASP E		82.521		102.438		. E
ATOM	7823	C	ASP E		80.511		102.438	1.00 49.83	. E
ATOM	7824	ō	ASP E						
ATOM	7825	N	ALA E		81.071		104.278	1.00 54.01	E
MOTA	7826	_			80.097		104.212	1.00 54.55	E
	7827	CA	ALA E		80.343		105.629	1.00 62.04	E
ATOM		CB	ALA E	•	79.149	42.097		1.00 59.72	E
MOTA	7828	C	ALA E		81.563	41.887	•	1.00 68.47	E
MOTA	7829	0	ALA E		82.299			1.00 68.58	E
ATOM	7830	N	THR E		81.767		104.707	1.00 77.30	E
ATOM	7831	CA	THR E		82.889		104.664	1.00 83.99	. E
ATOM	7832	CB	THR E		82.808	39.197	103.431	1.00 80.64	E
MOTA	7833	OG1	THR E	71	83.982	38.378	103.385	1.00 80.75	E
MOTA	7834	CG2			82.685		102.135	1.00 80.44	E
MOTA	7835	C	THR E		84.212	40.893		1.00 90.60	E
ATOM	7836	ō	THR E		84.633	41.417		1.00 93.08	E
ATOM	7837	N	ASN E		84.854	40.949		1.00 94.55	E
MOTA	7838	CA	ASN E		86.136	41.626		1.00 99.52	B
ATOM	7839	CB	ASN E			. 41.670		1.00105.13	E
				. ,	50.555	,			

MOTA	7840	CG	ASN	Ė	72	85.841	42.761	108.198	1.00110.92	E
MOTA	7841	OD1	ASN	E	72	86.064	42 924	109.403	1.00111.97	E
ATOM	7842		ASN		72			•		
-						84.983		107.516	1.00112.48	E
MOTA	7843	С	ASN		72	87.221	40.932	105.112	1.00100.12	E
ATOM	7844	0	ASN	E	72	88.146	40.326	105.660	1.00101.78	·E
ATOM	7845	N	ASN	E	73	87.101	41.022	103.789	1.00 98.06	E
ATOM	7846	CA	ASN		73	88.069		102.883		
									1.00 94.81	E
MOTA	7847	CB	ASN		73	89.339		102.813	1.00 96.94	E
MOTA	7848	CG	ASN	E	73	89.041	42.761	102.748	1.00 97.49	E
ATOM	7849	OD1	ASN	E	73	88.508	43.345	103.695	1.00 96.53	E
ATOM	7850	MD2	ASN	E	73	89.387		101.628	1.00 95.84	E
ATOM	7851	C	ASN		73					
						88.437		103.354	1.00 90.62	E
ATOM	7852	0	ASN		73	89.587		103.231	1.00 90.22	E
MOTA	7853	N	GLN	E	74	87.460	38.280	103.902	1.00 85.30	E
ATOM	7854	CA	GLN	E	74	87.682	36.919	104.395	1.00 80.03	E
ATOM	7855	CB	GLN	E	74	86.814	36 667	105.638	1.00 84.73	Ē
ATOM	7856	CG	GLN		74	87.144				
								106.809	1.00 92.54	E
ATOM	7857	CD	GLN		74	86.059		107.889	1.00 94.84	E
ATOM	7858	OE1	GLN	E	74	86.204	38.395	108.887	1.00 92.19	E
MOTA	7859	NE2	GLN	E	74	84.970	36.936	107.690	1.00 92.52	E
ATOM	7860	С	GLN	E	74	87.359		103.306	1.00 72.13	Ē
ATOM	7861	ō	GLN		74	87.261		103.568		
									1.00 69.91	E.
MOTA	7862	N	LEU		75	87.202	_	102.080	1.00 63.45	E
ATOM	7863	CA	LEU	\mathbf{E}	75	86.881	35.546	100.935	1.00 58.02	E
MOTA	7864	CB	LEU	E.	75	85.776	36.189	100.087	1.00 46.47	E
ATOM	7865	CG	LEU	E	75	84.403		100.705	1.00 42.52	E
ATOM	7866		LEU		75	83.636	37.399	99.843		
									1.00 34.46	E
ATOM	7867	-	LEU	_	75	83.652		100.867	1.00 38.91	E
MOTA	7868	C	LEU		75	88.100	35.347	100.050	1.00 59.56	E
ATOM -	7869	0	LEU	E	75	89.051	36.126	100.100	1.00 62.69	E
ATOM	7870	N	PRO	E	76	88.088	34.295	99.222	1.00 58.52	E
MOTA	7871	CD	PRO		76	87.078	33.226	99.151	1.00 58.84	
										E
ATOM	7872	CA	PRO		76	89.206	34.019	98.318	1.00 59.64	E
ATOM	7873	CB	PRO	E	76	88.682	32.858	97.484	1.00 58.08	E
MOTA	7874	CG	PRO	\mathbf{E}	76	87.834	32.120	98.452	1.00 55.57	E
MOTA	7875	С	PRO	E	76	89.479	35.267	97.466	1.00 62.30	E
MOTA	7876	0	PRO		76	88.537	35.919	97.012	1.00 60.80	E
ATOM	7877	N	GLN		77					
						90.752	35.596	97.247	1.00 63.51	Ε
	7878	CA	GLN		77	91.100	36.780	96.467	1.00 62.98	E
ATOM	7879	CB	GLN	Е	77 ·	92.145	37.599	97.217	1.00 61.45	· E
MOTA	7880 4	CG	GLN	\mathbf{E}	77	91.627	38.142	98.526	1.00 67.26	E
MOTA	7881	CD	GLN	E	77	90.368	38.967	98.342	1.00 72.26	E
ATOM	7882		GLN		77	89.380	38.786	99.063		
									1.00 68.32	
MOTA	7883.		GLN		77	90.398	39.886	97.376	1.00 72.34	E
MOTA	7884	C	GLN	E	77	91.578	36.522	95.039	1.00 63.00	· E
ATOM	7885	0	GLN	E	77	91.914	37.459	94.316	1.00 63.48	E
ATOM	7886	N	ASP	Е	78	91.586	35.260	94.628	1.00 60.29	E
MOTA	7887	CA	ASP		78	92.026	34.907	93.289	1.00 58.86	
										E
MOTA	7888	CB	ASP		78	92.912	33.659	93.344	1.00 57.86	E
MOTA	7889	CG	ASP		78	92.222	32.477	94.001	1.00 60.35	E
MOTA	7890	OD1	ASP	E	78	92.697	31.338	93.826	1.00 66.03	E
MOTA	7891		ASP		78	91.210	32.675	94.702	1.00 63.50	E
ATOM	7892	C	ASP		78	90.860	34.652	92.333	1.00 60.14	
										E
ATOM	7893	0	ASP		78	91.033	34.610	91.113	1.00 61.33	E
MOTA	7894	N	ARG		79	89.664	34.496	92.886	1.00 59.24	E
MOTA	7895	CA	ARG	E	79	88.499	34.199	92.070	1.00 53.51	E
MOTA	7896	CB	ARG		79	88.288	32.692	92.051	1.00 55.18	E
ATOM	7897	CG	ARG		79	87.959	32.121	93.427	1.00 59.32	
	1031	<u> </u>	Auc	***		01.939	JE . LEL	JJ.44/	1.00 37.32	E

MOTA	7898	CD	ARG	E 7	9	88.185	30.629	93.479	1.00	60.46	E
MOTA	7899	NE	ARG		9	89.613	30.351	93.415	1.00	67.44	E
MOTA	7900	CZ	ARG	E 7	9	90.140	29.149	93.219	1.00	66.77	E
MOTA	7901	NH1	ARG	E 7	9	89.355	28.088	93.066	1.00	63.21	E
MOTA	7902	NH2	ARG	E 7	9	91.458	29.014	93.173	1.00	67.67	E
ATOM	7903	C	ARG	E 7	9	87.274	34.854	92.652	1.00	47.91	E
ATOM	7904	0	ARG	E 7	9	87.308	35.349	93.770		47.61	E
MOTA	7905	N	GLU	E 8	0	86.186	34.847	91.893		45.69	E
ATOM	7906	CA	GLU		0 .	84.936	35.425	92.373		41.83	E
MOTA	7907	CB	GLU		0	83.953	35.661	91.232		36.72	Ē
ATOM	7908	CG	GLU		0	84'.422	36.479	90.068		34.45	E
ATOM	7909	CD	GLU		0	83.322	36.623	89.031		36.06	E
ATOM	7910		GLU		0	82.824	37.753	88.819		25.44	E
MOTA	7911	OE2			0	82.939	35.590	88.439		41.97	E
ATOM	7912	C	GLU		0	84.289	34.413	93.316		42.04	E
ATOM	7913	ō	GLU		0	84.536	33.205	93.221		40.99	E
ATOM	7914	N	SER		1	83.459	34.906	94.224		38.94	E
ATOM	7915	CA	SER		1	82.754	34.024	95.129		37.54	E
ATOM	7916	CB	SER		1	83.036	34.404	96.579		36.16	E
ATOM	7917	OG	SER		1	84.421	34.275	96.866		46.69	
ATOM	7918	C	SER		1	81.287	34.201	94.787		37.57	E
ATOM	7919	Ö	SER		1	80.821	35.326		-		E
ATOM	7920	N	LEU		2	80.562	33.094	94.602 94.672		39.92	E
ATOM	7921	CA	LEU		2	79.145	33.153	94.330		37.80 37.09	E
ATOM	7922	CB	LEU		2	78.725	31.859	93.632			E
ATOM	7923	CG	LEU		2	77.230	31.579	93.465		33.42 36.62	E E
ATOM	7924		LEU		2	76.479	32.766	92.888		36.62	E
ATOM	7925		LEU		2	77.089	30.387	92.576		34.16	E
ATOM	7926	C	LEU		2	78.234	33.404	95.523		37.97	· B
ATOM	7927	ŏ.	LEU		2	78.371	32.766	96.572		36.17	E
ATOM	7928	N	PHE		3	77.308	34.345	95.350	-	36.70	B
ATOM	7929	CA	PHE		3	76.334	34.683	96.383		36.32	E
ATOM	7930	CB			3	76.724	35.955	97.122		34.64	E
ATOM	7931	CG			3	77.841	35.765	98.093		38.99	E
ATOM	7932				3	79.162	35.718	97.657		29.61	E
ATOM	7933		PHE		3	77.571	35.603	99.455		41.22	E
ATOM	7934				3	80.198	35.508	98.556		26.15	E
ATOM	7935				3	78.606		100.364		34.51	E
MOTA	7936	CZ			3	79.924	35.346	99.906		34.28	E
MOTA	7937 [.]	C			3	74.974	34.892	95.743		35.98	Ē
MOTA	7938	0		-	3	74.881	35.054	94.535		35.96	Ē
MOTA	7939	N			4	73.921	34.891	96.557		33.53	· E
MOTA	7940	CA	TRP		4	72.593	35.085	96.034		27.70	E
MOTA	7941	CB			4	71.794	33.794	96.124		21.62	E
ATOM	7942	CG	TRP		4	72.352	32.728	95.250		22.88	E
ATOM	7943	CD2	TRP		4	72.049	32.491	93.865		15.47	Ē
MOTA	7944	CE2	TRP	-	4	72.827	31.390	93.450		17.90	E
MOTA	7945		TRP		4	71.202	33.101	92.938		21.85	E
MOTA	7946	CD1	TRP		4	73.274	31.795	95.601		26.81	E
MOTA	7947		TRP		4	73.563	30.981	94.528		24.54	E
MOTA	7948		TRP		4	72.782	30.886	92.146		17.47	E
MOTA	7949	CZ3	TRP		4	71.154	32.600	91.644	1.00	9.99	E
MOTA	7950		TRP		4	71.937	31.507	91.262		17.03	E
MOTA	7951	C	TRP		4	71.860	36.206	96.725		31.06	E
MOTA	7952	0	TRP	-	4	71.710	36.216	97.946		35.05	E
MOTA	7953	N	MET		5	71.404	37.143	95.900		29.79	E
ATOM	7954	CA	MET		5	70.674	38.332	96.300		26.47	E
MOTA	7955	CB	MET		5	71.093	39.468	95.358		24.99	E
					-						~

ATOM	7956	CG	MET	E 8	85	70.302	40.755	95.472	1.00	29.53	E
ATOM	7957	SD	MET	F 1	85	70.743	41.719	96.891		40.16	E
	7958										
ATOM		CE	MET		85	69.573	43.093	96.778		28.55	E
MOTA	7959	С	MET	E	85	69.163	38.042	96.200	1.00	27.49	E
MOTA	7960	0	MET	E	85	68.664	37.582	95.159	1.00	26.09	E
ATOM	7961	N	ASN	E S	86	68.442	38.308	97.289	1.00	27.72	E
ATOM	7962	CA	ASN		36	66.999	38.064	97.346		25.63	Ē
MOTA	7963	CB	ASN		B6	66.677	36.922	98.341		22.17	E
ATOM	7964	CG	asn	E 8	B 6	67.237	35.562	97.896	1.00	26.58	E
ATOM	7965	ODI	ASN	E 8	36	68.420	35.260	98.092	1.00	27.53	E
ATOM	7966	MD3	ASN	R 8	36	66.385	34.743	97.294		18.64	E
ATOM	7967	C	ASN		86	66.235	39.319	97.741		23.31	E
ATOM	7968	0	ASN		36	66.601	39.994	98.683		28.66	E
ATOM	7969	N	VAL		87	65.174	39.625	97.005	1.00	24.58	E
MOTA	7970	CA	VAL		87	64.344	40.798	97.264	1.00	21.63	E
ATOM	7971	CB	VAL	E 8	37	64.541	41.888	96.177	1.00	21.57	E
ATOM	7972	CG1	VAL		37	63.643	43.079	96.444		11.14	E
ATOM	7973	CG2	VAL		37	66.008	42.338	96.144			
										13.01	E
MOTA	7974	С	VAL		37 ·	62.918	40.283	97.234	1.00	24.89	E
ATOM	7975	0	VAL	E 8	3 7	62°. 406	39.854	96.196	1.00	21.75	E
MOTA	7976	N	LYS	E 8	88	62.310	40.320	98.414	1.00	27.63	E
ATOM	7977	CA	LYS	E S	88	60.961	39.847	98.658		30.74	E
ATOM	7978	CB	LYS		38	60.950	39.114	99.988		27.69	
											E
MOTA	7979	CG	LYS		88	59.625		100.467		30.49	E
ATOM	7980	CD	LYS	E 8	38	59.869	37.532	101.466	1.00	32.98	E
ATOM	7981	CE	LYS	E 8	38	58.690	37.316	102.378	1.00	39.50	E
ATOM	7982	NZ	LYS	E 8	38	59.099	36.365	103.432	1.00	41.12	E
	7983	C	LYS		38		40.982	98.687		32.94	E
			LYS				42.027				
MOTA	7984	0			38	60.236	_	99.270		36.53	E
ATOM	7985	N	ALA		39	58.807	40.778	98.052	1.00	32.23	E
MOTA	7986	CA.	ALA	E 8	39 .	57.768	41.797	98.031	1.00	34.52	E
MOTA	7987	CB .	ALA	E 8	3 9	57.294	42.036	96.619	1.00	38.48	E
ATOM	7988	C	ALA	E 8	39	56.612	41.327	98.892		36.68	E
ATOM	7989	ō	ALA		39	55.813	40.489	98.481		37.19	E
ATOM	7990	N	ILE		90	56.525		100.094		39.91	E
ATOM	7991	CA	ILE		90	55.472	41.498	101.023	1.00	43.86	E
MOTA	7992	CB	ILE	E 9	90	55.944	41.669	102.481	1.00	41.73	E
MOTA	7993	CG2	ILE	E 9	90	54.807	41.348	103.435	1.00	37.50	E
ATOM	7994	CG1	ILE	E 9	90	57.153	40.770	102.749	1.00	41.42	E
ATOM	7995	CD1	ILE		90	57.772		104.123		36.06	Ē
ATOM		C	ILE								
	7996				90	54.195		100.839		49.62	E
MOTA	7997	0	ILE		90	54.196		100.973		53.43	E.
ATOM	7998	N	PRO	E S	91	53.080	41.646	100.528	1.00	50.88	E
MOTA	7999	CD	PRO	E S	91	52.876	40.228	100.200	1.00	47.40	E
ATOM	8000	CA	PRO	E 9	91	51.846	42,405	100.356	1.00	52.77	E
ATOM	8001	CB	PRO		91	50.930	41.410	99.667		43.99	E
	8002	CG	PRO								
ATOM					91	51.373		100.231		47.25	E
ATOM	8003	C	PRO		91	51.332		101.722		58.30	E
MOTA	8004	0	PRO	E S	91	52.105	43.050	102.651	1.00	59.29	E
ATOM	8005	N	SER	E :	92	50.026	43.012	101.842	1.00	66.75	E
ATOM	8006	CA	SER		92	49.423		103.092		70.53	E
ATOM	8007	CB	SER		92					71.10	E
						49.103		102.993			
ATOM	8008	OG	SER		92	48.760		101.652		72.77	E
MOTA	8009	C	SER		92	48.163	42.625	103.309	1.00	74.39	E
MOTA	8010	0	SER	E !	92	47.531	42.217	102.342	1.00	78.28	E
ATOM	8011	N	MET		93	47.798		104.563		79.36	E
ATOM	8012	CA	MET		93	46.609		104.869		84.73	Ē
ATOM		CB						104.883			_
MIOM	8013	CB	MET	 :	93	46.667	41.0/3	100.323	T.00	90.59	. E

ATOM	8014	CG	MET	E	93		45.718	39.902	106.647	1.00 99.54	E
MOTA	8015	'sd	MET	E	93		44.009	40.307	107.183	1.00107.95	В
ATOM	8016	CE	MET		93		43.997		108.839	1.00102.16	B
ATOM	8017	C	MET		93		45.304				
					_				104.646	1.00 85.19	E
ATOM	8018	0	MET		93		45.100		105.218	1.00 83.73	E
MOTA	8019	N	ASP		94		44.431	41.786	103.802	1.00 87.08	E
ATOM	8020	CA	ASP	Е	94		43.135	42.404	103.536	1.00 87.83	E
ATOM	8021	CB	ASP	Е	94		42.395	41.739	102.363	1.00 88.98	E
ATOM	8022	CG	ASP	E	94		43.155	41.815	101.051	1.00 93.19	E
ATOM	8023	OD1	ASP	R	94		42.492	41.873	99.988	1.00 89.53	E
ATOM	8024		ASP		94		44.405		101.076	1.00 .95.08	E
ATOM	8025	C	ASP		94		42.290		104.776		
										1.00 87.87	E
MOTA	8026	0	ASP		94		42.071		105.189	1.00 86.91	E
MOTA	8027	N	LYS		95		41.828		105.384	1.00 89.56	E
MOTA	8028	CA	LYS		95		40.972		106.552	1.00 89.71	E
ATOM	8029	CB	LYS	Е	95		40.931	44.464	107.327	1.00 89.46	E
ATOM	8030	CG	LYS	B	95		42.221	44.798	108.058	1.00 87.67	E
MOTA	8031	CD	LYS	E	95		43.332	45.235	107.129	1.00 90.85	E
ATOM	8032	CE	LYS	E	95		43.085	46.633	106.578	1.00 90.41	E
ATOM	8033	NZ	LYS		95		44.257		105.806	1.00 90.02	Ē
ATOM	8034	C	LYS		95		39.601		105.973	1.00 90.47	E
ATOM	8035	ō	LYS	_	95		38.619		106.692	1.00 90.02	
ATOM	8036		SER		96						E
		Ŋ					39.574		104.648	1.00 92.81	E
ATOM	8037	CA	SER		96		38.369		103.878	1.00 93.23	E
MOTA	8038	CB	SER		96		38.459		102.501	1.00 92.72	E
MOTA	8039	OG	SER		96		39.652	42.728	101.817	1.00 90.65	E
ATOM	8040	С	SER	E	96	٠.	38.074	40.916	103.686	1.00 93.41	E
MOTA	8041	0	SER	Е	96		36.907	40.513	103.646	1.00 94.89	. E
ATOM	8042	N	LYS	E	97		39.116	40.099	103.551	1.00 91.56	E
ATOM	8043	CA	LYS	E	97		38.923		103.355	1.00 90.60	E
ATOM	8044	CB	LYS		97		39.802		102.208	1.00 92.72	Ē
MOTA	8045	CG	LYS		97		39.782		100.953	1.00 97.27	E
ATOM	8046	CD	LYS		97						
							38.398		100.337	1.00102.20	E
ATOM	8047	CE	LYS		97		38.419	40.032	99.108	1.00105.13	E
ATOM	8048	NZ	LYS		97		37.056	40.261	98.549	1.00106.19	E
MOTA	8049	C	LYS		97		39.273		104.636	1.00 88.83	E
MOTA	8050	0	LYS		97		39.449	36.700	104.635	1.00 88.67	E
ATOM	8051	N	LEU		98		39.353	38.670	105.726	1.00 87.92	E
ATOM	8052	CA	LEU	E	98		39.697	38.159	107.049	1.00 88.15	E
ATOM	8053	CB	LEU	E	98		39.498	39.290	108.069	1.00 91.70	E
ATOM	8054	CG	LEU	E	98		39.764	39.077	109.563	1.00 94.58	E
ATOM	8055	CD1	LEU	E	98		38.557	38.427	110.209	1.00 93.87	E
ATOM	8056	CD2	LEU	E	98		41.027		109.756	1.00 95.95	E
ATOM	8057	C	LEU		98		38.989		107.522	1.00 86.75	E
ATOM	8058	ō	LEU		98		39.641		108.076	1.00 86.39	E
ATOM	8059	N	THR		99		37.673	_	107.319	1.00 84.26	E
		CA							-		_
ATOM	8060		THR		99		36.917		107.746	1.00 81.01	E
ATOM	8061	CB	THR		99		35.512		108.291	1.00 84.06	E
MOTA	8062		THR		99		34.695		107.216	1.00 85.84	E
ATOM	8063	CG2	THR		99		35.609	37.025	109.385	1.00 79.28	E
MOTA	8064	C	THR		99		36.726	34.652	106.569	1.00 78.00	E
ATOM	8065	0	THR	E	99		35.733	33.930	106.477	1.00 75.16	E
MOTA	8066	N	GLU		100		37.690		105.661	1.00 77.82	E
ATOM	8067	CA	GLU				37.647		104.478	1.00 76.57	Ē
ATOM	8068	CB	GLU				37.577		103.222	1.00 79.22	E
MOTA	8069	CG	GLU				36.223		102.979	1.00 79.22	E
ATOM	8070	CD	GLU						102.979		
MOTA							36.250			1.00 85.86	E
MION	8071	ÓRI	GLU	Ľ	T00		36.732	30.004	100.743	1.00 88.66	E

MOTA	8072	OE2	GLU		100	35.783	37.496	102.046	1.00 87	7.70	E
MOTA	8073	C	GLU	E	100	38.864	32.942	104.380	1.00 72		E
MOTA	8074	0	GLU	Е	100	39.874	33.168	105.039	1.00 72	2.40	E
MOTA	8075	N	asn	E	101	38.750	31.912	103.555	1.00 70	0.72	E
MOTA	8076	CA	ASN	Е	101	39.853	31.000	103.319	1.00 68	3.45	E
MOTA	8077	CB	ASN	Е	101	39.324	29.650	102.860	1.00 69	9.36	E
MOTA	8078	CG	ASN	E	101	39.153	28.687	104.008	1.00 72	2.47	E
ATOM	8079	OD1	ASN	E	101	38.993	29.101	105.162	1.00 70	0.21	E
MOTA	8080	ND2	ASN	E	101	39.186	27.393	103.705	1.00 71		E
MOTA	8081	Ć.	ASN	E	101	40.654	31.661	102.221	1.00 65	5.35	E
MOTA	8082	0	ASN	E	101	40.173		101.093	1.00 64		E
ATOM	8083	N	THR	E	102	41.871		102.551	1.00 61		Е
MOTA	8084	CA	THR	E	102	42.706	32.783	101.585	1.00 58		E
MOTA	8085	CB	THR	E	102	42.834	34.260	101.977	1.00 59		E
ATOM	8086	OG1	THR	Ε	102	43.418		103.282	1.00 65		Ē
MOTA	8087	CG2	THR	E	102	41.471	34.923	102.014	1.00 63	3.21	E
MOTA	8088	С	THR	Е	102	44.112	32.250	101.376	1.00 53		E
ATOM	8089	0	THR	E	102	44.652	31.497	102.193	1.00 46	5 . 83	E
ATOM	8090	N	LEU	E	103	44.686		100.245	1.00 53		E
ATOM	8091	CA	LEU			46.060	32.287	99.894	1.00 52		E
ATOM	8092	CB	LEU	Е	103	46.137	31.252	98.766	1.00 47		E
ATOM	8093	CG	LEU			47.580	31.081	98.263	1.00 45		E
ATOM	8094	CD1	LEU		103	48.432	30.438	99.373	1.00 48		E
ATOM	8095	CD2	LEU	E	103	47.611	30.240	97.010	1.00 42		E
ATOM	8096	С	LEU			46.771	33.531	99.412	1.00 50		·E
ATOM	8097	0	LEU	E	103	46.315	34.195	98.484	1.00 49		E
ATOM	8098	N	GLN			47.882		100.046	1.00 51		E
ATOM	8099	CA	GLN			48.629	35.017	99.595	1.00 49		- E
ATOM	8100	CB	GLN			48.733		100.697	1.00 52		E
ATOM	8101	CG ·	GLN	E	104	47.932		100.364	1.00 52		E
ATOM	8102	CD			104	48.101	_	101.385	1.00 52		E
MOTA	8103		GLN			47.562		101.220	1.00 50		E
ATOM	8104	NE2				48.852		102.447	1.00 49		E
MOTA	8105	C	GLN			50.010	34.602	99.131	1.00 45		E
ATOM	8106	0	GLN			50.643	33.724	99.721	1.00 42		E
ATOM	8107	N	LEU			50.461	35.218	98.050	1.00 40		E
ATOM	8108	CA	LEU			51.777	34.919	97.539	1.00 38		Ē
ATOM	8109	CB	LEU			51.726	34.674	96.036	1.00 37		E
MOTA	8110	CG	LEU			50.889	33.484	95.566	1.00 36		E
MOTA	8111	CD1	LEU			51.067	33.328	94.077	1.00 39		E
MOTA	8112	CD2				51.321	32.210	96.266	1.00 43		E
MOTA	8113	C	LEU			52.683	36.102	97.826	1.00 35		E
MOTA	8114	0	LEU			52.223	37.221	97.961	1.00 39		E
ATOM	8115	N	ALA			53.970	35.825	97.956	1.00 34		E
MOTA	8116	CA	ALA			54.989	36.836	98.187	1.00 28		E
ATOM	8117	CB	ALA	E	106	55.600	36.680	99.576	1.00 24		E
ATOM	8118	C	ALA			56.036	36.559	97.116	1.00 29		E
MOTA	8119	0	ALA			56.761	35.551	97.161	1.00 31	55	E
MOTA	8120	N	ILE			56.100	37.435	96.129	1.00 29		E
MOTA	8121	CA	ILE			57.055	37.250	95.056	1.00 25		E
MOTA	8122	CB	ILE			56.688	38.085	93.838	1.00 24		E
MOTA	8123	CG2				57.473	37.585	92.622	1.00 26		E
ATOM	8124		ILE			55.190	37.966	93.559	1.00 22		E
ATOM	8125		ILE			54.765	36.580	93.092	1.00 23		E
ATOM	8126	C	ILE			58.425	37.680	95.528	1.00 27		Ē
MOTA	8127	ō	ILE			58.569	38.671	96.254	1.00 29		E
MOTA	8128	N	ILE			59.433	36.933	95.106	1.00 28		Ē
MOTA	8129	CA	ILE			60.808	37.239	95.465	1.00 30		E

MOTA	8130	CB	ILE	E	108	61.363	36.201	96.470	1.00 31.17	E
MOTA	8131	CG2	ILE	E	108	62.770	36.590	96.903	1.00 20.29	E
MOTA	8132	CG1	ILE	E	108	60.403	36.068	97.661	1.00 28.26	E
MOTA	8133	CD1	ILE	E	108	60.653	34.821	98.509	1.00 19.06	E
ATOM	8134	С	ILE	E	108	61.660	37.171	94.206	1.00 29.17	E
MOTA	8135	0	ILE	E	108	61.420	36.331	93.337	1.00 27.52	E
MOTA	8136	N	SER	E	109	62.644	38.054	94.097	1.00 29.12	E
ATOM	8137	CA	SER	E	109	63.542	38.007	92.945	1.00 28.65	E
ATOM	8138	CB	SER	E	109	63.652	39.378	92.282	1.00 25.60	E
ATOM	8139	OG	SER	E	109	62.372	39.852	91.889	1.00 29.24	E
ATOM	8140	C	SER	E	109	64.870	37.593	93.566	1.00 28.87	E
MOTA	8141	0	SER	E	109	65.300	38.181	94.563	1.00 30.52	E
ATOM	8142	N	ARG			65.477	36.545	93.021	1.00 24.79	E
MOTA	8143	CA	ARG	E	110	66.746	36.039	93.521	1.00 27.37	E
MOTA	8144	CB	ARG	E	110	66.601	34.599	94.047	1.00 25.59	Ē
ATOM	8145	CG	ARG	E	110	67.849	33.730	93.788	1.00 30.47	E
ATOM	8146	CD	ARG	E	110	67.781	32.339	94.401	1.00 23.46	E
MOTA	8147	NE	ARG	E	110	67.741	32.440	95.852	1.00 29.94	E
ATOM	8148	CZ	ARG	E	110	68.591	31.850	96.686	1.00 29.72	E
MOTA	8149	NH1	ARG	E	110	69.578	31.085	96.237	1.00 16.98	E
MOTA	8150	NH2	ARG	E	110	68.458	32.061	97.984	1.00 24.90	E
ATOM	8151	C	ARG	E	110	67.747	36.060	92.375	1.00 33.03	E
MOTA	8152	0	ARG	E	110	67.583	35.347	91.373	1.00 31.91	E
ATOM	8153	N	ILE	E	111	68.791	36.871	92.533	1.00 34.02	E
MOTA	8154	CA	ILE	E	111	69.807	36.984	91.505	1.00 31.29	E
MOTA	8155	CB	ILE	E	111	69.737	38.356	90.859	1.00 32.17	E
ATOM	8156	CG2	ILE	E	111	68.370	38.535	90.181	1.00 32.88	E
MOTA	8157	CG1	ILE		111	69.967	39.428	91.920	1.00 32.03	E
MOTA	8158	CD1	ILE	E	111	70.100	40.828	91.349	1.00 27.85	E
MOTA	8159	C	ILE		111	71.217	36.746	92.018	1.00 27.76	E
MOTA .	8160	0	ILE	E	111	71.495	36.905	93.201	1.00 29.85	E
MOTA	8161	N	LÝS	E	112	72.109	36.363	91.118	1.00 26.03	E
MOTA	8162	CA	LYS	Е	112	73.487	36.115	91.494	1.00 28.03	E
MOTA	8163	CB	LYS	E	112	74.249	35.460	90.353	1.00 26.10	E
MOTA	8164	CG	LYS	E	112	73.547	34.310	89.684	1.00 28.45	E
ATOM	8165	CD	LYS	Е	112	74.371	33.862	88.492	1.00 35.18	E
MOTA	8166	CE	LYS	E	112	73.690	32.776	87.701	1.00 44.85	E
MOTA	8167	NZ	LYS	E	112	74.524	32.371	86.528	1.00 45.06	E
MOTA	8168	C	LYS	E	112	74.198	37.413	91.855	1.00 27.69	E
ATOM	8169	0	LYS	E	112	73.945	38.468	91.292	1.00 32.27	E
ATOM	8170	N	LEU	E	113	75.086	37.321	92.819	1.00 26.20	E
MOTA	8171	CA	LEU	E	113	75.868	38.452	93.244	1.00 30.07	E
ATOM	8172	CB	LEU	E	113	75.437	38.903	94.633	1.00 26.50	E
MOTA	8173	CG	LEU	E	113	76.385	39.835	95.386	1.00 28.06	E
ATOM	8174	CD1	LEU	E	113	76.998	40.835	94.438	1.00 40.23	E
ATOM	8175	CD2	LEU	E	113	75.614	40.573	96.457	1.00 34.89	E
ATOM	8176	С	LEU	E	113	77.290	37.912	93.277	1.00 35.19	E
MOTA	8177	0	LEU			77.567	36.962	94.011	1.00 43.89	E
ATOM	8178	N	TYR	E	114	78.180	38.461	92.458	1.00 30.39	E
MOTA	8179	CA	TYR	E	114	79.548	37.973	92.492	1.00 34.53	E
MOTA	8180	CB	TYR			80.130	37.763	91.091	1.00 31.04	E
ATOM	8181	CG	TYR			79.407	36.767	90.235	1.00 29.75	E
MOTA	8182		TYR			78.646	37.187	89.145	1.00 27.37	E
ATOM	8183		TYR			77.976	36.281	88.353	1.00 23.53	Ē
ATOM	8184		TYR			79.482	35.405	90.504	1.00 28.01	E
ATOM	8185		TYR			78.814	34.480	89.706	1.00 25.24	E
ATOM	8186	CZ	TYR			78.063	34.931	88.636	1.00 27.63	E
ATOM	8187	OH	TYR			77.384	34.042	87.839	1.00 33.91	E

MOTA	8188	С	TYR E	114	80.448	38.949	93.221	1.00 38.12	E
MOTA	8189	0	TYR E	114	80.372	40.166	93.021	1.00 38.72	E
ATOM	8190	N	TYR E		81.289	38.403	94.083	1.00 40.23	E
MOTA	8191	CA	TYR E		82.269	39.194	94.802	1.00 41.88	E
ATOM	8192	CB	TYR E		82.583	38.541	96.143	1.00 40.46	Ē
ATOM	8193	CG	TYR E		83.665	39.239	96.912	1.00 45.20	Ē
ATOM	8194	CD1			83.418	40.468	97.531	1.00 47.84	E
ATOM	8195	CE1	TYR E		84.402	41.123	98.248	1.00 47.84	E
ATOM	8196	CD2	TYR E		84.941	38.678	97.030	1.00 43.74	E
ATOM	8197	CE2	TYR E		85.940	39.326	97.747		
ATOM	8198	CZ	TYR E					1.00 46.84	E
ATOM		OH			85.664 86.644	40.552	98.355	1.00 51.90	E
	8199		TYR E			41.217	99.060	1.00 57.44	E
ATOM	8200	C	TYR E		83.458	39.035	93.859	1.00 43.51	E
ATOM	8201	0			83.998	37.939	93.717	1.00 47.45	E
ATOM	8202	N	ARG E		83.847	40.105	93.182	1.00 46.54	E
ATOM	8203	CA	ARG E		84.960	40.022	92.244	1.00 48.67	E
ATOM	8204	CB	ARG E		84.577	40.676	90.916	1.00 50.62	E
MOTA	8205	CG	ARG E		85.669	40.636	89.855	1.00 55.10	E
ATOM	8206	CD	ARG E		85.126	41.074	88.506	1.00 48.73	E
ATOM	8207	NE	ARG E		84.197	40.087	87.974	1.00 49.25	E
ATOM	8208	CZ	ARG E		83.268	40.353	87.063	1.00 47.27	E
ATOM	8209		ARG E		83.150	41.583	86.590	1.00 45.04	B
ATOM	8210		ARG E		82.462	39.390	86.623	1.00 44.03	E
MOTA	8211	C	ARG E		86.217	40.667	92.783	1.00 50.92	E
ATOM	8212	0	ARG E		86.341	41.885	92.792	1.00 51.75	E
ATOM	8213	N	PRO E	•	87.168	39.851	93.252	1.00 56.58	E
MOTA	8214	CD	PRO E		87.192	38.379	93.241	1.00 58.31	E
MOTA	8215	CA	PRO E		88.422	40.387	93.790	1.00 62.30	E
ATOM	8216	CB	PRO E		89.293	39.141	93.956	1.00 59.71	E
MOTA	8217	CG	PRO E		88.303	38.073	94.223	1.00 59.53	E
MOTA	8218	C	PRO E		89.007	41.346	92.771	1.00 65.34	E
MOTA	8219	0	PRO E		89.511	40.920	91.742	1.00 67.65	E
ATOM	8220	N	ALA E		88.916	42.637	93.040	1.00 71.43	E
ATOM	8221	CA	ALA E		89.451	43.623	92.115	1.00 77.39	E
ATOM	8222	CB	ALA E		88.963	45.025	92.504	1.00 82.03	E
ATOM	8223	C	ALA E		90.977	43.555	92.154	1.00 79.41	E
MOTA	8224	0	ALA E		91.606	44.229	92.974	1.00 79.28	E
ATOM	8225	N	LYS E		91.559	42.737	91.270	1.00 80.34	E
ATOM	8226	CA	LYS E		93.011	42.559	91.194	1.00 79.09	E
ATOM	8227	CB	LYS E		93.580	42.328	92.596	1.00 79.93	E
ATOM	8228	CG	LYS E		95.067	42.627	92.749	1.00 82.41	E
MOTA	8229	CD	LYS E		95.339	44.119	92.887	1.00 81.91	E
MOTA	8230	CE	LYS E		96.767	44.373	93.376	1.00 84.83	E
MOTA	8231	NZ	LYS E		97.051	45.806	93.688	1.00 86.64	E
MOTA	8232	С	LYS E		93.362	41.357	90.311	1.00 79.42	E
ATOM	8233	0	LYS E		94.475	40.829	90.375	1.00 80.69	E
MOTA	8234	N	LEU E		92.418	40.929	89.482	1.00 78.31	E
MOTA	8235	CA	LEU E		92.639	39.773	88.617	1.00 76.92	E
MOTA	8236	CB	TEA E		91.326	39.011	88.435	1.00 78.87	E
ATOM	8237	CG	LEU E		90.520	38.821	89.725	1.00 78.12	E
MOTA	8238		LEU E		89.227	38.091	89.422	1.00 77.81	E
ATOM	8239		LEU E		91.345	38.056	90.745	1.00 77.20	E
MOTA	8240	C	LEU E		93.195	40.176	87.258	1.00 75.89	E
MOTA	8241	0	LEU E		92.919	41.271	86.759	1.00 75.25	E
MOTA	8242	N	ALA E		93.974	39.278	86.660	1.00 74.37	E
MOTA	8243	CA	ALA E		94.595	39.537	85.363	1.00 71.38	E
ATOM	8244	CB	ALA E		95.741	38.557	85.135	1.00 71.37	E
MOTA	8245	C	ALA E	121	93.609	39.451	84.210	1.00 67.34	E

MOTA	8246	0	ALA :	B 121	93.230	40.456	83.621	1.00 65.61	E
MOTA	8247	N	LEU	E 122	93.201	38.235	83.891	1.00 66.30	E
MOTA	8248	CA	LEU :	E 122	92.273	38.009	82.802	1.00 67.41	E
ATOM	8249	CB		E 122	91.902	36.529	82.756	1.00 67.53	E
ATOM	8250	CG	LEU		90.736	36.126	81.856	1.00 71.32	Ē
ATOM	8251		LEU :		90.764	36.927	80.566	1.00 69.46	. E
MOTA	8252	CD2	LEU :		90.817	34.628	81.584	1.00 72.73	E
MOTA	8253	C		E 122	91.017	38.858	82.907	1.00 67.54	E
MOTA	8254	0	LEU :	E 122	90.185	38.629	83.768	1.00 70.87	E
ATOM	8255	N	PRO :	E 123	90.860	39.848	82.018	1.00 68.07	E
MOTA	8256	CD	PRO :	E 123	91.771	40.218	80.920	1.00 69.16	B
MOTA	8257	CA	PRO 1	E 123	89.680	40.721	82.033	1.00 68.69	E
ATOM	8258	CB		E 123	90.065	41.822	81.048	1.00 69.48	E
ATOM	8259	CG		E · 123	90.884	41.084	80.039	1.00 69.70	E
		C			88.397				
ATOM	8260			E 123		39.973	81.623	1.00 67.34	E
ATOM	8261	0	PRO 1		88.363	39.288	80.599	1.00 67.21	E
MOTA	8262	N.		E 124	87.325	40.117	82.416	1.00 64.53	E
MOTA	8263	CD	PRO 1	E 124	87.209	41.151	83.453	1.00 63.28	E
MOTA	8264	CA	PRO 1	E 124	86.026	39.476	82.191	1.00 63.28	E
ATOM	8265	CB	PRO 1	3 124	85.050	40.370	82.966	1.00 62.47	E
MOTA	8266	CG	PRO 1	E 124	85.817	41.631	83.226	1.00 65.30	E
MOTA	8267	C	PRO 1	E 124	85.604	39.259	80.742	1.00 63.28	Ē
ATOM	8268	ō		E 124	85.061	38.208	80.395	1.00 60.22	E
ATOM	8269	N	ASP I		85.842	40.250	79.899	1.00 66.27	E
ATOM			ASP 1						
	8270	CA			85.491	40.146	78.485	1.00 71.14	. E
ATOM	8271	CB	ASP I		85.960	41.398	77.772	1.00 77.36	E
MOTA	8272	CG	ASP I		87.425	41.673	78.028	1.00 84.23	E
MOTA	8273		ASP 1		88.286	40.920	77.517	1.00 86.56	E
MOTA	8274	OD2	ASP 1	E 125	87.720	42.635	78.764	1.00 90.78	E
ATOM	8275	C	ASP I	3 125	86.184	38.947	77.843	1.00 72.05	E
MOTA	8276	0	ASP 1	3 125	85.633	38.271	76.972	1.00 71.71	E
ATOM	8277	N	GLN I	3 126	87.406	38.704	78.294	1.00 72.31	E
ATOM	8278	CA	GLN I		88.257	37.644	77.780	1.00 74.02	Ē
ATOM	8279	CB	GLN I		89.702	38.172	77.843	1.00 79.69	E
ATOM	8280	CG	GLN I		90.810				
						37.336	77.190	1.00 86.00	E
ATOM	8281	CD	GLN I		92.171	38.029	77.289	1.00 87.14	E
ATOM	8282		GLN I		93.222	37.417	77.062	1.00 87.09	E
MOTA	8283	NE2			92.150	39.318	77.624	1.00 86.89	E
MOTA	8284	C	GLN I		88.111	36.305	78.527	1.00 72.95	E
MOTA	8285	0	GLN 1	E 126	89.083	35.560	78.665	1.00 74.41	E
ATOM	8286	N	ALA 1	3 127	. 86.903	35.984	78.991	1.00 70.16	E
ATOM	8287	CA	ALA 1	3 127	86.692	34.742	79.739	1.00 65.81	E
MOTA	8288	CB	ALA 1	E 127	85.986	35.044	81.050	1.00 59.82	E
MOTA	8289	C	ALA I		85.956	33.622	78.997	1.00 64.60	E
ATOM	8290	Ō		E 127	86.378	32.469	79.040	1.00 63.08	: E
MOTA	8291	N		3 128	84.866	33.948	78.315	1.00 64.06	E
ATOM	8292	CA		3 120 3 128	84.109				
						32.932	77.590	1.00 66.61	E
MOTA	8293	CB		E 128	82.996	33.589	76.788	1.00 62.84	E
ATOM	8294	C		E 128	84.992	32.080	76.665	1.00 70.89	E
MOTA	8295	0	ALA :		84.826	30.859	76.587	1.00 70.48	E
MOTA	8296	N		E 129	85.930	32.726	75.976	1.00 74.32	E
MOTA	8297	CA	GLU I	E 129	86.837	32.047	75.050	1.00 75.77	E
MOTA	8298	CB		E 129	87.841	33.033	74.472	1.00 81.67	E
MOTA	8299	CG		E 129	87.390	34.477	74.491	1.00 97.61	E
MOTA	8300	CD		E 129	88.565	35.447	74.471	1.00103.11	E
MOTA	8301	OE1			88.331	36.664	74.278	1.00103.11	E
MOTA	8302		GLU :	- 120 - 120	89.719	34.990			
							74.662	1.00104.91	E
ATOM	8303	C	الالك	E 129	87.631	30.942	75.730	1.00 75.65	E

ATOM	8304	0	GLU E	129	87.826	29.863	75.163	1.00 76.89	E
ATOM	8305	N	LYS E		88.108	31.231	76.938	1.00 71.46	Ē
ATOM	8306	CA	LYS E		88.911	30.288	77.703	1.00 68.34	E
MOTA	8307	CB	LYS E		89.385	30.939	79.002	1.00 72.68	E
ATOM	8308	CG	LYS E		90.110	32.270	78.817		
ATOM	8309	CD	LYS E					1.00 76.69	. E
					91.477	32.083	78.179	1.00 78.95	E
ATOM	8310	CE	LYS E		92.154	33.415	77.900	1.00 80.02	E
MOTA	8311	NZ	LYS E		93.512	33.220	77.309	1.00 80.28	E
MOTA	8312	C	LYS E	•	88.170	29.007	78.038	1.00 66.39	E
MOTA	8313	0	LYS E		88.742	28.104	78.641	1.00 66.28	E
ATOM	8314	N	LEU E		86.904	28.926	77.642	1.00 64.93	E
ATOM	8315	CA	LEU E	131	86.092	27.751	77.928	1.00 66.19	E
MOTA	8316	CB	LEU E	131	84.604	28.070	77.781	1.00 63.41	E
ATOM	8317	CG	LEU E	131	83.700	26.931	78.275	1.00 59.42	E
MOTA	8318	CD1	LEU E	131	83.805	26.830	79.799	1.00 54.50	E
ATOM	8319	CD2	LEU E	131	82.267	27.178	77.850	1.00 56.06	E
ATOM	8320	C	LEU E		86.398	26.557	77.049	1.00 69.57	· E
ATOM	8321	0	LEU E		86.045	26.544	75.873	1.00 74.49	E
MOTA	8322	N	ARG E		87.031	25.544	77.624	1.00 72.41	E
ATOM	8323	CA	ARG E		87.357	24.336	76.877	1.00 78.60	E
ATOM	8324	CB	ARG E		88.748	23.836		1.00 78.60	
ATOM	8325	CG	ARG E				77.273		E
ATOM					89.846	24.882	77.138	1.00 89.83	E
	8326	CD	ARG E		91.098	24.466	77.907	1.00 96.13	E
ATOM	8327	NE	ARG E		91.968	25.607	78.196	1.00100.26	E
ATOM	8328	CZ	ARG E		93.006	25.569	79.029	1.00101.37	E
MOTA	8329		ARG E		93.316	24.443	79.664	1.00100.07	E
ATOM	8330		ARG E		93.727	26.664	79.239	1.00102.77	E
MOTA	8331	C	ARG E	- '	86.305	23.268	77.180	1.00 79.65	E
ATOM	8332	0	ARG E		85.317	23.539	77.863	1.00 78.67	E
MOTA	8333	N	PHE E	133	86.511	22.055	76.678	1.00 81.70	E
MOTA	8334	CA	PHE E	133	85.555	20.979	76.912	1.00 86.89	E
ATOM	8335	CB	PHE E	133	84.550	20.906	75.759	1.00 86.42	E
MOTA	8336	CG	PHE E	133	83.637	22.090	75.674	1.00 86.29	E
ATOM	8337	CD1	PHE E	133	84.110	23.320	75.237	1.00 86.42	E
MOTA	8338	CD2	PHE E	133	82.304	21.981	76.057	1.00 88.13	E
ATOM	8339	CEl	PHE E		83.272	24.427	75.182	1.00 88.07	E
MOTA	8340	CE2			81.453	23.078	76.008	1.00 88.03	E
ATOM	8341	CZ	PHE E		81.937	24.307	75.570	1.00 88.68	E
ATOM	8342	c	PHE E	133	86.168	19.595	77.126	1.00 91.17	E
ATOM	8343	ō	PHE E		87.358	19.452	77.412	1.00 93.88	E
ATOM	8344	N	ARG E		85.321	18.581	76.985	1.00 93.88	E
ATOM	8345	CA	ARG E		85.689	17.178			
MOTA			ARG E				77.148	1.00 95.08	E
ATOM	8346	CB			86.147	16.903	78.575	1.00 91.89	E
	8347	CG	ARG E		86.322	15.433	78.889	1.00 91.75	E
ATOM	8348	CD	ARG E		86.312	15.220	80.391	1.00 95.21	E
ATOM	8349	NE	ARG E		87.383	15.960	81.052	1.00 98.21	E
MOTA	8350	CZ	ARG E		87.388	16.268	82.345	1.00 99.25	E
MOTA	8351		ARG E		86.372	15.903	83.119	1.00 98.61	E
MOTA	8352	NH2	ARG E		88.410	16.938	82.866	1.00 99.33	E
ATOM	8353	C.	ARG E		84.399	16.421	76.871	1.00 99.10	. E
MOTA	8354	0	ARG E		83.615	16.149	77.786	1.00100.13	E
ATOM	8355	N	ARG E	135	84.183	16.077	75.606	1.00101.44	E
MOTA	8356	ÇA	ARG E		82.954	15.404	75.209	1.00101.64	Ē
MOTA	8357	CB	ARG E		82.405	16.077	73.955	1.00101.47	E
ATOM	8358	CG	ARG E	•	83.232	15.842	72.712	1.00 99.48	Ē
ATOM	8359	CD	ARG E		82.414	15.023	71.762	1.00101.08	E
ATOM	8360	NE	ARG E		81.112	15.649	71.587	1.00 99.91	E
ATOM	8361	CZ	ARG E		80.032	15.017	71.152	1.00 99.63	E
					55.052			x.00 JJ.03	17

ATOM	8362	NH1	ARG F	135		78.890	15.678	71.027	1.00101.44	E
MOTA	8363	NH2	ARG E	135		80.090	13.726	70.853	1.00 99.66	E
MOTA	8364	C	ARG I			83.025	13.902	74.978	1.00101.20	E
MOTA	8365	ō	ARG I			83.717	13.437	74.075	1.00101.89	E
MOTA	8366	М	SER E			82.296	13.153	75.802	1.00100.13	E
ATOM	8367	CA	SER I			82.230	11.700	75.678	1.00100.13	E
MOTA	8368	CB	SER E			82.123	11.037	77.059	1.00100.33	E
ATOM	8369	OG	SER E			83.346	11.115	77.775	1.00 99.88	E
ATOM	8370	C	SER E			80.988	11.374	74.847	1.00102.00	E
MOTA	8371	0	SER E			80.686	12.066	73.872	1.00101.18	E
ATOM	8372	N	ALA F	–		80.274	10.321	75.229	1.00103.10	E
MOTA	8373	CA	ALA E	137		79.058	9.932	74.525	1.00105.11	E
ATOM	8374	CB	ALA E	137		79.166	8.490	74.049	1.00103.80	E
MOTA	8375	С	ALA E	3 137		77.895	10.084	75.498	1.00106.97	· E
ATOM .	8376	0	ALA E	137		76.781	9.619	75.242	1.00107.91	E
ATOM	8377	N	ASN E	138		78.177	10.749	76.617	1.00107.06	E
ATOM	8378	CA	ASN E			77.190	10.970	77.665	1.00106.52	E
ATOM	8379	CB	ASN E			76.861	9.640	78.356	1.00107.20	Ē
ATOM	8380	CG	ASN E			78.108	8.826	78.699	1.00106.89	E
ATOM	8381		ASN E			79.019	9.295	79.395	1.00102.98	·E
MOTA	8382		ASN E			78.146	7.593	78.208	1.00102.38	
ATOM	8383	C	ASN E			77.643	11.977	78.719	1.00103.22	E
			ASN E							E
MOTA	8384	0				76.824	12.534	79.448	1.00103.13	E
MOTA	8385	N	SER E			78.944	12.228	78.789	1.00104.04	E
MOTA	8386	CA	SER E		•	79.458	13.137	79.802	1.00102.32	E
MOTA	8387	CB	SER E			80.227	12.326	80.848	1.00102.39	E
MOTA	8388	OG	SER E			79.468	11.202	81.265	1.00104.25	E
MOTA	8389	C	SER E			80.329	14.296	79.316	1.00100.91	E
ATOM	8390	0	SER F			81.551	14.275	79.493	1.00101.38	E
ATOM	8391	N	LEU E	140		79.702	15,305	78.711	1.00 97.48	E
ATOM	8392	CA	LEU E	140		80.418	16.489	78.240	1.00 91.39	E
MOTA	8393	CB	LEU E	140		79.530	17.298	77.301	1.00 89.73	E
MOTA	8394	CG	LEU E	140		80.225	18.400	76.501	1.00 91.43	E
ATOM	8395	CD1	LEU E			79.189	19.146	75.669	1.00 89.37	E
MOTA	8396		LEU E		-	80.952	19.352	77.441	1.00 93.09	E
ATOM	8397	C	LEU E			80.734	17.313	79.491	1.00 88.57	E
ATOM	8398	ō	LEU E			79.837	17.651	80.260	1.00 91.20	E
ATOM	8399	N	THR E			81.998	17.655	79.688	1.00 84.25	E
ATOM	8400	CA	THR E			82.381	18.388	80.884	1.00 81.72	E
MOTA	8401	CB	THR E			83.426	17.569	81.687	1.00 81.72	E
MOTA	8402	OG1				82.877	16.283	82.005	1.00 78.08	
MOTA	8403	CG2	THR E			83.812				E
							18.291	82.985	1.00 82.28	E
ATOM	8404	C	THR E			82.915	19.807	80.683	1.00 81.01	E
ATOM	8405	0	THR E			84.119	19.999	80.473	1.00 81.29	E
ATOM	8406	N	LEU E			82.021		80.771	1.00 77.33	E
MOTA	8407	CA	LEU E			82.408	22.200	80.633	1.00 73.34	E
MOTA	8408	CB	TEA E			81.257	23.129	81.034	1.00 66.84	E
MOTA	8409	CG	LEU E			79.865	23.111	80.376	1.00 70.30	E
MOTA	8410		LEU E			79.897	23.800	79.028	1.00 66.49	E
MOTA	8411	CD2	LEU E			79.350	21.682	80.265	1.00 67.38	E
MOTA	8412	C	LEU E			83.585	22.425	81.584	1.00 73.42	E
ATOM	8413	0	LEU E	142		83.553	21.991	82.734	1.00 72.01	E
ATOM	8414	N	ILE E			84.627	23.091	81.106	1.00 74.59	E
MOTA	8415	CA	ILE E			85.801	23.340	81.936	1.00 74.87	E
MOTA	8416	CB	ILE E			86.975	22.436	81.493	1.00 75.32	E
ATOM	8417		ILE E			86.905	22.206	80.001	1.00 76.40	E
ATOM	8418	CGI	ILE E	3 143		88.316	23.047	81.907	1.00 72.09	E
ATOM	8419	CD1	ILE E			88.549	23.068	83.402	1.00 78.40	E
						50.545	25.000	33.702	/0.40	تر

MOTA	8420	C	ILE	E	143	86.218	24.803	81.879		74.98	E
MOTA	8421	0	ILE			86.581	25.316	80.824	1.00	76.39	E
MOTA	8422	N	ASN	E	144	86.167	25.464	83.031	1.00	73.35	E
ATOM	8423	CA	ASN	E	144	86.516	26.877	83.140	1.00	71.60	E
MOTA	8424	CB	ASN		144	85.314	27.658	83.676	1.00	68.98	E
MOTA	8425	CG	asn	Е	144	85.647	29.088	84.017	1.00	68.58	E
MOTA	8426	OD1	ASN	E	144	86.716	29.590	83.669	1.00	67.82	E
ATOM	8427	ND2	ASN			84.723	29.761	84.699	1.00	66.54	E
ATOM	8428	C	ASN	E	144	87.731	27.098	84.033	1.00	70.36	E
MOTA	8429	0	ASN	E	144	87.678	26.868	85.237	1.00	70.48	E
MOTA	8430	N	PRO	E	145	88.849	27.547	83.440	1.00	70.94	E
ATOM	8431	CD	PRO	E	145	89.052	27.526	81.977	1.00	71.02	E
MOTA	8432	CA	PRO	E	145	90.118	27.816	84.129	1.00	70.41	E
ATOM	8433	CB	PRO	E	145	91.150	27.442	83.079	1.00	70.45	E
ATOM	8434	CG	PRO	E	145	90.496	27.977	81.829	1.00	71.57	E
ATOM	8435	C	PRO	E	145	90.295	29.258	84.588	1.00	69.07	E
ATOM	8436	0	PRO	E	145	91.235	29.570	85.318	1.00	71.53	E
MOTA	8437	N	THR	E	146	89.402	30.136	84.148	1.00	66.19	E
ATOM	8438	CA	THR	E	146	89 [{] .472	31.549	84.510	1.00	61.24	E
MOTA	8439	CB	THR	E	146	88.520	32.361	83.641	1.00	59.37	E
ATOM	8440	OG1	THR	E	146	87.252	32.462	84.291		51.21	E
MOTA	8441	CG2	THR	E	146	88.321	31.672	82.293	1.00	57.20	E
ATOM	8442	C	THR			89.061	31.726	85.966	1.00	61.91	· E
ATOM	8443	0	THR			88.882	30.751	86.685	1.00	66.35	E
ATOM	8444	N	PRO	E	147	88.942	32.973	86.433		60.67	E
ATOM	8445	CD	PRO		147	89.738	34.128	85.984		62.20	E
ATOM	8446	CA	PRO	B	147	88.535	33.161	87.827	1.00	58.61	E
ATOM	8447	CB	PRO		147	89.584	34.120	88.349	1.00	60.83	E
ATOM	8448	CG	PRO			89.695	35.061	87.202		62.62	E
ATOM	8449	C	PRO			87.128	33.752	87.925		55.62	. E
ATOM	8450	0	PRO	E	147	86.787	34.388	88.921	1.00	53.78	E
ATOM	8451	N	TYR	E	148	86.322	33.546	86.886	1.00	54.39	E
MOTA	8452	CA	TYR			84.952	34.061	86.862		55.56	E
ATOM	8453	CB	TYR			84.749	35.068	85.726		54.28	E
MOTA	8454	CG	TYR			85.758	36.172	85.657		58.80	E
ATOM	8455	CD1	TYR			87.038	35.948	85.148		58.71	E
ATOM	8456	CE1	TYR			87.975	36.976	85.093	1.00	59.11	E
ATOM	8457	CD2	TYR			85.439	37.450	86.105		62.41	E
ATOM	8458	CE2	TYR		148	86.370	38.486	86.055		62.49	E
ATOM	8459	CZ	TYR			87.634	38.241	85.552		61.63	E
MOTA	8460	OH	TYR		148	88.557	39,262	85.549		69.01	E.
ATOM	8461	C	TYR		148	83.917	32.954	86.665	1.00	54.44	E
MOTA	8462	0	TYR		148	84.180	31.946	86.005		55.52	E
ATOM	8463	N	TYR		149	82.730	33.150	87.227		48.91	Е
ATOM	8464	CA	TYR			81.683	32.166	87.053		45.60	E
ATOM	8465	CB	TYR			80.530	32.406	88.044		43.27	E
ATOM	8466	CG	TYR			80.707	31.732	89.380	1.00	43.34	E
ATOM	8467	CD1				81.479	32.310	90.383		46.33	E
ATOM	8468	CE1				81.688	31.654	91.606		45.08	E
ATOM	8469		TYR			80.140	30.483	89.629		49.19	E
ATOM	8470	CE2				80.344	29.816	90.852		44.11	E
ATOM	8471	CZ	TYR			81.117	30.405	91.832		42.23	Ē
ATOM	8472	OH	TYR			81.316	29.755	93.032		37.45	E
ATOM	8473	C	TYR			81.180	32.283	85.612		43.17	Ē
ATOM	8474	Õ	TYR			80.794	33.360	85.163		44.66	E
ATOM	8475	N	LEU			81.183	31.175	84.884		38.35	E
ATOM	8476	CA	LEU			80.712	31.217	83.518		34.91	Ē
ATOM	8477	CB	LEU			81.624	30.388	82.602		35.61	E
				_			55.000				_

ATOM	8478	CG	LEU E	150	83.083	30.868	82.453	1.00 43.21	E
ATOM	8479	CD1	LEU E	150	83.796	29.992	81.450	1.00 47.59	E
ATOM	8480	CD2	LEU E	150	83.141	32.321	81.980	1.00 41.17	Е
ATOM	8481	C	LEU E	150	79.291	30.721	83.431	1.00 35.54	E
ATOM	8482	0	LEU E	150	78.985	29.571	83.763	1.00 35.91	E
ATOM	8483	N	THR E		78.406	31.604	82.999	1.00 35.55	E
MOTA	8484	CA	THR E		77.019	31.225	82.854	1.00 38.94	E
ATOM	8485	CB	THR E		76.059	32.399	83.192	1.00 38.59	E
ATOM	8486	OG1			76.294	32.849	84.531	1.00 36.43	E
ATOM	8487	CG2			74.606	31.947	83.078	1.00 39.58	E
ATOM	8488	C	THR E		76.835	30.800	81.405	1.00 43.18	E
ATOM	8489	Ö	THR E		76.833	31.591	80.561	1.00 47.17	E
ATOM	8490	N	VAL E		77.179	29.549	81.124	1.00 47.17	E
ATOM	8491	CA	VAL E		77.052	28.981	79.789	1.00 49.06	E
MOTA	8492	CB	VAL E		77.826	27.652	79.676	1.00 43.00	E
MOTA			VAL E		77.525	26.972	78.362	1.00 51.19	E
	8493		VAL E						E
ATOM	8494				79.327	27.904	79.796	1.00 49.69	
ATOM	8495	C	VAL E		75.595	28.703	79.448	1.00 51.18	E
ATOM ·		0	VAL E		74.922	27.954	80.146	1.00 53.77	· E
ATOM	8497	N	THR E		75.121	29.315	78.372	1.00 54.28	E
ATOM	8498	CA	THR E		73.754	29.129	77.913	1.00 58.13	E
ATOM	8499	CB	THR E		72.910	30.389	78.208	1.00 57.51	E
MOTA	8500		THR E		71.546	30.185	77.796	1.00 55.66	E
MOTA	8501	CG2			73.498	31.589	77.487	1.00 55.49	E
MOTA	8502	C	THR E		73.785	28.842	76.400	1.00 62.76	E
MOTA	8503	0	THR E		74.827	29.006	75.744	1.00 61.22	E
MOTA	8504	N	GLU E		72.646	28.408	75.858	1.00 66.49	E
MOTA	8505	CA	GLU E		72.517	28.069	74.438	1.00 68.76	E
ATOM	8506	CB	GLU E		72.501	29.333	73.578	1.00 66.26	E
ATOM .	8507	CG	GLU E	154	71.261	30.172	73.775	1.00 72.22	E
MOTA	8508	CD	GLU E		71.010	31.117	72.619	1.00 78.23	E
MOTA	8509	OE1	GLU E	154	70.010	31.874	72.661	1.00 78.16	E
MOTA	8510	OE2			71.813	31.096	71.662	1.00 84.45	E
ATOM	8511	С	GLU E	154	73.629	27.135	73.974	1.00 71.00	E
MOTA	8512	0	GLU E	154	74.212	27.315	72.904	1.00 72.26	E
ATOM	8513	И.	LEU E	155	73.917	26.133	74.796	1.00 73.04	E
MOTA	8514	CA	LEU E	155	74.947	25.150	74.492	1.00 75.03	E
MOTA	8515	CB	LEU E	155	75.376	24.425	75.768	1.00 69.28	E
MOTA	8516	CG	LEU E	155	76.563	23.472	75.659	1.00 64.86	E
MOTA	8517	CD1	LEU E	155	77.823	24.263	75.323	1.00 64.88	E
MOTA	8518	CD2	LEU E	155	76.740	22.732	76.971	1.00 63.06	E
ATOM	8519	C	LEU E	155	74.370	24.143	73.510	1.00 80.05	E
MOTA	8520	0	LEU E	155	73.184	23.815	73.575	1.00 79.70	E
ATOM	8521	N	ASN E	156	75.207	23.645	72.605	1.00 85.84	E
MOTA	8522	CA	ASN E	156	74.748	22.677	71.617	1.00 89.34	E
MOTA	8523	CB	ASN E	156	74.198	23.415	70.406	1.00 87.22	E
MOTA	8524	CG	ASN E	156	73.216	24.489	70.796	1.00 90.32	E.
ATOM	8525		ASN E		72.145	24.198	71.324	1.00 93.80	E
MOTA	8526		ASN' E		73.581	25.745	70.559	1.00 92.39	E
MOTA	8527	C	ASN E		75.855	21.729	71.185	1.00 92.87	E
MOTA	8528	ō	ASN E		76.995	22.148	70.966	1.00 91.78	E
ATOM	8529	N	ALA E		75.506	20.448	71.079	1.00 97.29	E
ATOM	8530	CA	ALA E		76.447	19.414	70.659	1.00101.18	E
ATOM	8531	CB	ALA E		75.943	18.043	71.095	1.00101.13	Ē
ATOM	8532	C	ALA E		76.549	19.480	69.139	1.00101.13	Ē
ATOM	8533	0	ALA E		76.729	18.465	68.462	1.00104.33	E
ATOM		Ŋ	GLY E		76.723	20.698	68.619	1.00105.98	E
	8534		GLY E		76.424	20.838	67.190	1.00108.48	E
MOTA	8535	CA	ת דותם	1 720	10.400	40.74	01.170	T.00T0/.5/	2

ATOM	8536	С	GLY H	158	75.101	21.234	66.663	1.00109.34	E
MOTA	8537	Ō	GLY F		74.864	22.310	66.110	1.00109.40	E
MOTA	8538	N	THR I		74.186	20.284	66.847	1.00111.07	Ē
ATOM	8539	CA	THR I		72.804	20.423	66.397	1.00112.63	E
ATOM	8540	CB	THR I		72.420	19.317	65.400	1.00112.03	
MOTA	8541	OG1			72.420	18.045			· E
ATOM		CG2					66.055	1.00114.77	E
	8542		THR I		73.362	19.319	64.202	1.00115.94	E
MOTA	8543	C	THR E		71.892	20.278	67.600	1.00113.37	E
MOTA	8544	0	THR		70.950	21.050	67.781	1.00113.17	E
MOTA		. N	ARG		72.186	19.269	68.414	1.00114.32	E
MOTA	8546	CA	ARG E		71.412	18.993	69.612	1.00115.70	E
MOTA	8547	CB	ARG E		71.904	17.697	70.263	1.00120.12	E
ATOM	8548	CG	ARG E		71.060	17.210	71.440	1.00127.73	E
MOTA	8549	CD	ARG E	160	69.765	16.535	70.973	1.00132.71	E
MOTA	8550	NE	ARG E	160	69.083	15.831	72.057	1.00137.48	E
MOTA	8551	CZ	ARG E	160	68.282	16.409	72.949	1.00137.60	Е
ATOM	8552	NH1	ARG E	160	68.042	17.715	72.889	1.00139.24	E
MOTA	8553	NH2	ARG E	160	67.742	15.683	73.921	1.00136.81	B
MOTA	8554	C	ARG E		71.564	20.150	70.596	1.00113.60	E
MOTA	8555	0	ARG E		72.660	20.680	70.787	1.00113.52	E
ATOM	8556	N	VAL E		70.455	20.542	71.210	1.00110.19	E
ATOM	8557	CA	VAL E		70.469	21.621	72.188	1.00107.35	E
ATOM	8558	CB	VAL E		69.206	22.507	72.166	1.00107.33	E
ATOM	8559		VAL E		67.946	21.664			
MOTA	8560		VAL E				72.276	1.00108.93	E
ATOM					69.271	23.646	73.075	1.00107.68	E
	8561	C	VAL E		70.532	21.017	73.589	1.00104.33	E
MOTA	8562	0	VAL E		69.769	20.108	73.923	1.00104.97	E
	8563	N	LEU E		71.441	21.522	74.412	1.00100.01	E
ATOM	8564	CA	LEU E		71.586	21.004	75.766	1.00 96.80	E
ATOM	8565	CB	TEA E		73.064	20.771	76.074	1.00 97.92	E
ATOM	8566	CG	LEU E		73.747	19.749	75.169	1.00 98.31	E
MOTA	8567		LEU E		75.191	19.552	75,610	1.00 97.42	E
MOTA	8568	CD2	LEU E	162	72.979	18.439	75.237	1.00 98.39	E
ATOM	8569	С	LEU E	162	70.973	21.872	76.863	1.00 93.12	E
ATOM	8570	0	LEU E	162	70.147	22.757	76.608	1.00 92.56	E
ATOM	8571	N	GLU E	163	71.392	21.603	78.094	1.00 87.79	E
ATOM	8572	CA	GLU E	163	70.898	22.333	79.246	1.00 82.65	E
MOTA	8573	CB	GLU E	163	70.487	21.341	80.332	1.00 85.22	E
ATOM	8574	CG	GLU E	163	69.640	21.933	81.440	1.00 90.62	E
MOTA	8575	CD	GLU E	163	68.706	20.907	82.053	1.00 91.02	E
MOTA	8576	OE1	GLU E	163	67.695	20.564	81.402	1.00 89.20	E
ATOM	8577	OE2	GLU E		68.987	20.436	83.178	1.00 93.62	E
ATOM	8578	C	GLU E		71.974	23.293	79.756	1.00 77.13	E
ATOM	8579	o	GLU E		73.156	22.933	79.861	1.00 76.00	E
MOTA	8580	N	ASN E		71.554	24.519	80.060	1.00 68.76	E
ATOM	8581	CA	ASN E		72.458	25.561	80.537	1.00 62.46	E
ATOM	8582	CB	ASN E		71.651	26.757	81.010	1.00 62.03	E
ATOM	8583	CG	ASN E		70.605	27.165	80.012	1.00 66.90	
ATOM	8584		ASN E		70.921	27.669		1.00 68.02	. E
MOTA	8585		ASN E				78.934		E
ATOM					69.342	26.938	80.356	1.00 73.37	E
	8586	C	ASN E		73.371	25.097	81.658	1.00 58.94	E
MOTA	8587	0	ASN E		73.071	24.145	82.371	1.00 60.17	E
MOTA	8588	N	ALA E		74.491	25.780	81.826	1.00 54.91	E
MOTA	8589	CA	ALA E		75.410	25.399	82.877	1.00 53.53	E
ATOM	8590	CB	ALA E		76.477	24.474	82.332	1.00 54.95	E
MOTA	8591	C	ALA E		76.048	26.614	83.498	1.00 53.05	· E
MOTA	8592	0	ALA E		76.126	27.676	82.879	1.00 52.33	E
MOTA	8593	N	LEU E	166	76.478	26.446	84.743	1.00 49.24	E

ATOM	8594	CA	LEU	E 166	77.131	27.503	85.485	1.00 44.72	E
MOTA	8595	CB		E 166	76.327	27.856	86.738	1.00 39.66	E
ATOM	8596	CG	LEU		76.968	28.874	87.688	1.00 45.21	Ē
MOTA	8597	CD1		E 166	77.152	30.220	86.972	1.00 39.91	E
MOTA	8598			B 166	76.094	29.044	88.909	1.00 40.37	E
ATOM	8599	С		E 166	78.472	26.907	85.854	1.00 42.70	E
ATOM	8600	Õ		E 166	78.556	26.042	86.709	1.00 43.32	E
ATOM	8601	N		E 167	79.530	27.355	85.196	1.00 43.34	E
ATOM	8602	CA	VAL		80.832	26.788	85.487	1.00 43.55	E
ATOM	8603	СВ	VAL		81.638	26.516	84.215	1.00 42.61	E
ATOM	8604		VAL		82.873	25.711	84.561	1.00 45.25	E
ATOM	8605		VAL		80.777	25.771	83.201	1.00 45.20	E
ATOM	8606	C	VAL		81.662	27.654	86.392	1.00 45.84	E
ATOM	8607	ō	VAL		82.086	28.748	86.020	1.00 48.46	E
ATOM	8608	N	PRO		81.920	27.157	87.602	1.00 47.47	E
ATOM	8609	CD	PRO		81.459	25.828	88.036	1.00 47.47	E
ATOM	8610	CA		E 168	82.702	27.803	88.656	1.00 49.69	E
ATOM	8611	СВ		E 168	82.636	26.790	89.790	1.00 49.05	E
ATOM	8612	CG	PRO		82.490	25.478	89.065	1.00 48.13	E
ATOM	8613	C	PRO		84.138	28.130	88.261	1.00 48.13	E
ATOM	8614	ŏ	PRO		84.733	27.451	87.431	1.00 53.52	E
ATOM	8615	N	PRO		84.713	29.180	88.866	1.00 56.85	E
ATOM	8616	CD		E 169	84.038	30.057	89.838	1.00 59.48	E
ATOM	8617	CA	PRO		86.083	29.645	88.622	1.00 59.66	E
ATOM	8618	CB	PRO		86.260	30.756	89.654	1.00 59.86	E
ATOM	8619	CG		E 169		31.315	89.775	1.00 62.59	E
ATOM	8620	C	PRO		87.089	28.527	88.841	1.00 62.59	E
ATOM	8621	ŏ		E 169	86.972	27.772	89.806	1.00 65.74	
ATOM `		N	MET		88.077	28.427	87.958	1.00 61.17	E
ATOM	8623	CA		E 170	89.096	27.396	88.080	1.00 58.16	E
ATOM	8624	CB		E 170	90.132	27.835	89.105	1.00 58.25	. E
ATOM	8625	CG	MET		90.950	29.007	88.618	1.00 70.37	E
ATOM	8626	SD		E 170	91.910	29.829	89.892	1.00 83.55	E
MOTA	8627	CE	MET		90.978	31.381	90.036	1.00 84.38	E
ATOM	8628	C		E 170	88.465	26.071	88.481	1.00 56.84	Ē
ATOM	8629	ō		E 170	89.014	25.323	89.288	1.00 56.41	E
ATOM	8630	N		E 171	87.299	25.799	87.907	1.00 54.79	E
ATOM	8631	CA		E 171	86.591	24.575	88.200	1.00 57.47	E
ATOM	8632	C		E 171	85.943	24.042	86.944	1.00 62.52	E
MOTA	8633	ō		E 171	86.310	24.442	85.840	1.00 64.05	E
ATOM	8634	N		E 172	84.970	23.151	87.103	1.00 65.70	Ē
MOTA	8635	CA	GLU		84.302	22.560	85.955		E
MOTA	8636	СВ		E 172	85.222	21.511	85.330	1.00 75.52	E
ATOM	8637	CG		E 172	85.828	20.545	86.341	1.00 79.82	E
ATOM	8638	CD		E 172	86.952	19.721	85.744	1.00 85.82	E
ATOM	8639	OE1		E 172	86.673	18.932	84.814	1.00 85.82	E
MOTA	8640			E 172	88.112	19.868	86.198	1.00 87.13	E
MOTA	8641	C		E 172	82.955	21.937	86.293	1.00 67.75	E
ATOM	8642	ō'		E 172	82.654	21.667	87.448	1.00 68.63	. E
ATOM	8643	N		E 173	82.154	21.702	85.262	1.00 67.64	Ē
ATOM	8644	CA		E 173	80.830	21.121	85.417	1.00 70.11	E
ATOM	8645	CB		E 173	79.778	22.230	85.407	1.00 67.59	E
ATOM	8646	OG		E 173	80.298	23.417	85.980	1.00 37.39	E
MOTA	8647	C		E 173	80.570	20.177	84.248	1.00 73.57	E
ATOM	8648	ŏ		E 173	81.030	20.426	83.130	1.00 72.53	E
ATOM	8649	N		E 174	79.829	19.103	84.496	1.00 76.59	E
ATOM	8650	CA		E 174	79.528	18.158	83.435	1.00 78.85	E
ATOM	8651	CB		E 174	80.004	16.759		1.00 76.70	E
					30.004		55.055	±.00 /0./0	11

MOTA	8652	C	ALA :	E 174	78.042	18.129	83.101	1.00 80.41	E
MOTA	8653	0	ALA	E 174	77.217	17.789	83.944	1.00 82.68	· E
ATOM	8654	N	VAL .	E 175	77.704	18.509	81.876	1.00 83.44	E
ATOM	8655	CA	VAL :	E 175	76.323	18.473	81.417	1.00 90.29	E
ATOM	8656	CB	VAL :	E 175	76.018	19.623	80.430	1.00 91.72	E
MOTA	8657	CGl	VAL 3	E 175	74.662	19.388	79.756	1.00 87.34	E
MOTA	8658	CG2	VAL :	E 175	76.027	20.969	81.142	1.00 93.34	E
MOTA	8659	С	VAL :	E 175	76.115	17.147	80.699	1.00 95.14	E
MOTA	8660	0	VAL :	E 175	76.955	16.740	79.897	1.00 96.50	E
MOTA	8661	N	LYS :	E 176	75.005	16.473	80.998	1.00 97.88	E
MOTA	8662	CA	LYS :	E 176	74.719	15.180	80.382	1.00101.17	E
MOTA	8663	CB	LYS :	B 176	73.330	14.668	80.77 7	1.00 99.65	E
MOTA	8664	CG	LYS 1	E 176	73.189	14.266	82.252	1.00101.69	E
MOTA	8665	CD	LYS :	E 176	73.270	15.474	83.198	1.00100.25	E
MOTA	8666	CE	LYS :	E 176	72.853	15.114	84.629	1.00 92.38	E
MOTA	8667	NZ	LYS I	E 176	73.712	14.037	85.201	1.00 84.47	E
ATOM	8668	С	LYS I	E 176	74.798	15.279	78.857	1.00105.86	E
ATOM	8669	0	LYS 1	E 176	74.010	15.985	78.230	1.00106.00	E
ATOM	8670	N	LEU I		75.761	14.569	78.271	1.00109.97	E
ATOM	8671	CA	LEU I	E 177	75.976	14.532	76.821	1.00113.55	E
MOTA	8672	CB	LEU 1	E 177	77.442	14.180	76.563	1.00111.13	E
ATOM	8673	CG	LEU !	E 177	78.005	14.236	75.140	1.00110.68	E
MOTA	8674		LEU 1		77.402	15.402	74.356	1.00109.76	E
MOTA	8675	CD2	TEO 1	E 177	79.528	14.389	75.214	1.00108.19	E
MOTA	8676	C	LEU 1	E 177	75.022	13.495	76.207	1.00116.96	E
MOTA	8677	0	LEU 1		75.188	12.289	76.394	1.00117.37	E
MOTA	8678	N		E 178	74.016	13.969	75.448	1.00119.88	E
MOTA	8679	CD		E 178	73.902	15.386	75.058	1.00120.42	E
MOTA	8680	CA		E 178	72.975	13.183	74.775	1.00122.91	E
ATOM	8681	CB	PRO 1	E 178	72.077	14.260	74.184	1.00120.33	E
MOTA	8682	CG	PRO 1	E 178	73.054	15.305	73.805	1.00122.24	E
MOTA	8683	C	PRO 1		73.379	12.150	73.722	1.00126.75	E
MOTA	8684	Ο .	PRO 1		72.601	11.236	73.422	1.00128.10	E
ATOM	8685	И.			74.575	12.292	73.158	1.00128.80	E
ATOM	8686	CA		E 179	75.077	11.383	72.116	1.00129.28	E
ATOM	8687	CB	SER I		74.844	9.911	72.502	1.00129.66	E
ATOM	8688	OG	SER 1		75.544	9.038	71.628	1.00128.71	E
MOTA	8689	C		E 179	74.528	11.675	70.711	1.00128.87	E
MOTA	8690	0		E 179	75.050	11.164	69.707	1.00128.52	B
ATOM	8691	N		E 180	73.462	12.477	70.649	1.00127.78	E
ATOM	8692	CA		E 180	72.880	12.925	69.372	1.00125.71	E
MOTA	8693	CB	ASP I		71.479	13.522	69.588	1.00124.59	E
ATOM	8694	CG	ASP I		70.483	12.516	70.119	1.00123.01	E
ATOM	8695		ASP 1		69.321	12.908	70.394	1.00122.29	E
MOTA	8696		ASP I		70.851	11.332	70.252	1.00121.06	E
ATOM	8697	C		E 180	73.865	14.034	69.007	1.00124.59	E
MOTA	8698	0		E 180	73.555	15.019	68.362	1.00122.89	E
MOTA	8699	N		E 181	75.073	13.791	69.492	1.00124.55	E
MOTA	8700	CA		E 181	76.270	14.608	69.423	1.00124.38	E
MOTA	8701	CB		E 181	77.423	13.771	69.866	1.00123.55	E
MOTA	8702	C		E 181	76.653	15.298	68.125	1.00124.78	E
MOTA	8703	0		E 181	. 75.821	15.684	67.298	1.00123.76	E
MOTA	8704	N		E 182	77.967	15.498	68.043	1.00125.49	E
MOTA	8705	CA		E 182	78.650	16.132	66.935	1.00127.02	E
ATOM	8706	C		E 182	80.070	16.339	67.429	1.00128.13	E
MOTA	8707	0		E 182	80.868	15.401	67.462	1.00129.50	E
ATOM	8708	N		E 183	80.354	17.565	67.842	1.00127.43	E
ATOM	8709	CA	SER 1	E 183	81.648	17.974	68.359	1.00125.46	E

ATOM	8710	CB	SER	E	183	82.801	17.262	67.658	1.00125.67	E
ATOM	8711	OG	SER	E	183	83.949	17.259	68.489	1.00126.90	E
ATOM	8712	C .	SER			81.659	19.442	68.001	1.00123.66	Ē
ATOM	8713	Õ			183	82.537	20.209	68.404	1.00122.44	E
ATOM	8714	N	ASN			80.651	19.813	67.217	1.00121.65	
ATOM	8715	CA			184	80.449	21.186			E
								66.782	1.00118.72	E
ATOM	8716	CB		-	184	79.452	21.235	65.610	1.00118.99	E
MOTA	8717	CG	ASN		184	79.138	22.657	65.161	1.00119.20	E
MOTA	8718		ASN		184	80.032	23.397	64.744	1.00119.22	E
MOTA	8719		ASN		184	77.865	23.045	65.249	1.00118.04	E
ATOM	8720	C	ASN	Ε	184	79.867	21.900	67.987	1.00115.53	E
ATOM	8721	0	ASN	E	184	78.908	22.671	67.877	1.00114.96	E
MOTA	8722	N	ILE	В	185	80.442	21.610	69.147	1.00112.17	E
MOTA	8723	CA	ILE	Е	185	79.983	22.220	70.382	1.00108.97	E
MOTA	8724	CB	ILE	Е	185	80.936	21.901	71.552	1.00106.93	E
ATOM	8725	CG2	ILE	Е	185	80.427	22.564	72.826	1.00108.27	E
ATOM	8726	CG1	ILE	E	185	81.023	20.385		1.00102.38	Ē
ATOM	8727	CD1	ILE		185	81.884	19.970	72.925	1.00100.01	E
ATOM	8728	C	ILE		185	79.868	23.737	70.204	1.00106.71	E
ATOM	8729	ŏ	ILE		185	80.812	24.403	69.776	1.00106.68	
ATOM	8730	N	THR		186	78.694	24.269	70.522		E
ATOM	8731	CA	THR		186			_	1.00102.01	E
MOTA						78.432	25.691	70.376	1.00 96.59	E
	8732	CB	THR		186	77.513	25.910	69.198	1.00 94.19	E
ATOM	8733	OG1			186	76.413	25.000	69.289	1:00 95.20	E
ATOM	8734	CG2	THR		186	78.246	25.641	67.912	1.00 95.63	E
MOTA	8735	C	THR		186	77.806	26.288	71.629	1.00 92.99	E
MOTA	8736	0	THR		186	76.958	25.661	72.273	1.00 91.83	E
ATOM	8737	N	TYR		187	78.211	27.510	71.969	1.00 87.88	E
ATOM	8738	CA	TYR		187	77.698	28.140	73.176	1.00 79.80	E
MOTA	8739	CB	TYR	E	187	78.435	27.570	74.374	1.00 74.43	E
ATOM	8740	CG	TYR	Ε	187	79.874	28.011	74.405	1.00 68.14	E
MOTA	8741	CD1	TYR	E	187	80.229	29.268	74.885	1.00 69.19	E
ATOM	8742	CE1	TYR	Е	187	81.545	29.695	74.885	1.00 67.19	E
MOTA	8743	CD2	TYR	E	187	80.878	27.189	73.925	1.00 70.36	E
ATOM	8744	CE2	TYR	E	187	82.203	27.607	73.919	1.00 70.04	E
ATOM	8745	CZ	TYR		187	82.526	28.861	74.402	1.00 67.80	E
ATOM	8746	OH	TYR			83.833	29.276	74.403	1.00 71.27	E
MOTA	8747	C	TYR			77.872	29.644	73.209	1.00 76.42	E
MOTA	8748	ō	TYR			78.769	30.194	72.575	1.00 78.21	E
ATOM	8749	N	ARG		188	77.015	30.295	73.982	1.00 78.21	
ATOM	8750	CA	ARG		188	77.083	31.738	74.188		E
ATOM	8751	CB	ARG		188	75.839	32.419		1.00 67.64	E
MOTA	8752	CG	ARG					73.611	1.00 69.25	E
						75.546	32.047	72.166	1.00 73.45	E
ATOM	8753	CD	ARG			74.194	32.565	71.713	1.00 72.84	E
MOTA	8754	NE	ARG			74.167	34.017	71.599	1.00 79.18	E
ATOM	8755	CZ	ARG			74.839	34.707	70.683	1.00 .82.45	E
ATOM	8756		ARG			75.594	34.073	69.797	1.00 83.73	E
MOTA	8757		ARG			74.750	36.031	70.647	1.00 83.44	E
ATOM	8758	С	ARG	E	188	77.086	31.830	75.719	1.00 62.29	E
ATOM	8759	0	ARG	E	188	76.856	30.819	76.390	1.00 62.83	E
MOTA	8760	N	THR	E	189	77.381	32.991	76.291	1.00 53.76	E
MOTA	8761	CA	THR			77.341	33.078	77.749	1.00 48.05	E
MOTA	8762	CB	THR	E	189	78.721	33.086	78.399	1.00 40.38	E
MOTA	8763	OG1				79.297	34.388	78.272	1.00 32.65	E
MOTA	8764		THR			79.605	32.041	77.771	1.00 36.01	E
MOTA	8765	Ċ	THR			76.624	34.331	78.190	1.00 30.01	E
ATOM	8766	Ö	THR			76.024	35.075	77.358	1.00 49.31	E
MOTA	8767	N	ILE			76.594	34.564	79.502	1.00 52.41	E
	,			_		, , , , , , , ,	クェ・コウエ	10.004	T.OO 44.30	

ATOM	8768	CA	ILE	E	190		75.914	35.734	80.019	1.00	40.50	E
ATOM	8769	CB	ILE						-			
					190		74.725	35.298	80.882		31.68	E
ATOM	8770	CG2	ILE	E	190		73.881	36.497	81.268	1.00	28.51	E
MOTA	8771	CG1	ILE	E	190		73.875	34.315	80.066	1.00	31.75	E
ATOM	8772	CD1			190		72.577					
_								33.905	80.682		26.13	· E
MOTA	8773	С	ILE	Е	190		76.907	36.619	80.773	1.00	45.23	E
MOTA	8774	0	ILE	E	190		77.490	36.218	81.787	1.00	48.10	E
ATOM	8775	N	ASN		191							
							77.111	37.825	80.247		43.17	E
MOTA	8776	CA	ASN	E	191		78.052	38.768	80.832	1.00	42.56	É
MOTA	8777	CB	ASN	E	191		78.583	39.717	79.765	1.00	44.01	E
ATOM	8778	CG	ASN		191							
							77.482	40.553	79.140		46.11	E
ATOM	8779	ODI	ASN	Е	191		76.658	41.165	79.837	1.00	46.43	E
ATOM	8780	ND2	ASN	E	191		77.463	40.586	77.822	1.00	46.59	E
ATOM	8781	C	ASN	E	191		77.468		81.945		41.73	E
ATOM	8782	0	ASN		191		76.253	39.642	82.171	1.00	43.47	E
MOTA	8783	N	ASP	Е	192		78.375	40.328	82.597	1.00	34.08	E
ATOM	8784	CA	ASP	E	192		78.076	41.212	83.697	1.00	30.90	E
MOTA	8785	CB	ASP				79.258					
								42.150	83.938		33.04	E
MOTA	8786	CG	ASP		192		80.517	41.422	84.397	1.00	37.46	E
MOTA	8787	OD1	ASP	E	192		81.475	42.114	84.790	1.00	35.45	E
MOTA	8788	002	ASP		192		80.556	40.174	84.369		41.56	E
MOTA	8789	С	ASP				76.836	42.059	83.500	1.00	34.39	E
MOTA	8790	0	ASP	E	192		76.302	42.602	84.465	1.00	36.04	E
MOTA	8791	N	TYR	E	193		76.367	42.188	82.265	1.00	36.79	E
ATOM	8792	CA	TYR		193		75.196					
								43.024	82.021		39.38	E
ATOM	8793	CB	TYR	E	193		75.481	44.011	80.895	1.00	39.88	E
ATOM	8794	CG	TYR	E	193		76.807	44.676	81.098	1.00	43.20	E
ATOM	8795	CD1	TYR	E	193		77.919	44.283	80.363		44.07	E
						٠						
ATOM	8796	CE1	TYR		193		79.173	44.832	80.612	T.00	49.04	E
ATOM	8797	CD2	TYR	Е	193		76.977	45.641	82.094	1.00	45.49	Ē
MOTA	8798.	CE2	TYR	E	193		78.226	46.197	82.354	1.00	47.91	E.
ATOM	8799	CZ	TYR				79.322					
								45.789	81.608		48.45	E
MOTA	8800	OH	TYR	E	193		80.559	46.346	81.851	1.00	49.86	. E
ATOM	8801	C	TYR	E	193		73.999	42.185	81.703	1.00	39.19	E
MOTA	8802	0	TYR	E	193		72.972	42.682	81.238		39.41	E
MOTA			GLY									
	8803	N			194		74.147	40.898	81.975		40.01	E
MOTA	8804	CA	GLY	Е	194		73.064	39.970	81.746	1.00	44.70	E
ATOM	8805	C	GLY	Е	194		72.773	39.937	80.278	1.00	46.02	E
ATOM	8806	0	GLY	E.	194		71.633	39.719	79.858		40.25	E
MOTA	8807	N	ALA		195		73.833	40.170	79.508	1.00	52.12	E
MOTA	8808	CA	ALA	Ε	195		73.760	40.184	78.056	1.00	55.14	E
MOTA	8809	CB	ALA	E	195		74.410	41.457	77.528	1.00	57.76	E
ATOM	8810	C	ALA		195		74.455	38.946	77.482		55.29	
												E
ATOM	8811	0	ALA	E	195		75.464	38.486	78.019	1.00	49.52	E
ATOM	8812	N	LEU	E	196		73.889	38.407	76.402	1.00	59.02	E
ATOM	8813	CA	LEU	E	196		74.437	37.227	75.738	1 00	60.62	E
				_								
ATOM	8814	CB	LEU				73.426	36.642	74.751		60.51	Ė
ATOM-	8815	CG	LEU	E	196		72.222	35.873	75.299	1.00	65.69	E
MOTA	8816	CD1	LEU	E	196		71,244	35.532	74.174	1.00	62.28	E
ATOM	8817		LEU				72.714	34.610	75.982		64.87	E
MOTA	8818	С	LEU				75.697	37.585	74.973		62.63	E
MOTA	8819	0	LEU	E	196		75.699	38.509	74.164.	1.00	66.96	E
ATOM	8820	N	THR				76.779	36.867	75.233		63.16	E
ATOM												
	8821	CA	THR				78.005	37.138	74.514		62.75	E
MOTA	8822	CB.	THR	Е	197		79.230	36.514	75.208	1.00	61.23	E
MOTA	8823	OG1	THR				79.143	35.081	75.165	1.00	57.40	E
ATOM	8824		THR				79.304	36.995	76.648		58.08	
									70.040			E
MOTA	8825	C	THR	ĸ	T9./		77.806	36.515	73.139	1.00	66.39	E

MOTA	8826	0	THR E	197	76.8	325 35	.803 7	2.905	1.00	63.48	E
MOTA	8827	N	PRO E	198	78.7	719 36	.788 7	2.202	1.00	69.71	E
MOTA	8828	CD	PRO E	198	79.8	398 37	.668 7	2.264	1.00	69.96	E
MOTA	8829	CA	PRO E	198	78.5	63 36	.208 7	0.869	1.00	72.15	E
MOTA	8830	CB	PRO E	198	79.5	35 37	.028 7	0.033	1.00	69.88	. B
MOTA	8831	CG	PRO E	198	80.6	345 37	.289 73	1.010	1.00	72.14	Е
MOTA	8832	C	PRO E	198	78.8	378 34	.712 7	0.847	1.00	74.56	E
MOTA	8833	0	PRO E	198	79.7	776 34	.241 7	1.558	1.00	75.65	E
MOTA	8834	N	LYS E	199	78.1	.24 33	.981 7	0.028	1.00	75.53	E
MOTA	8835	CA	LYS E	199	78.2	72 32	.536 6	9.859	1.00	74.73	E
MOTA	8836	CB	LYS E	199	77.3	43 32	.077 6	8.736	1.00	73.23	E
MOTA	8837	CG	LYS E	199	77.4	67 30	.631 6	8.310	1.00	80.01	E
MOTA	8838	CD	LYS E	199	76.3	05 30	.309 6	7.362	1.00	86.06	E
MOTA	8839	CE	LYS E	199	76.5	82 29	.118 60	6.443	1.00	90.81	E
MOTA	8840	NZ	LYS E	199	. 76.7	45 27	.832 6	7.166	1.00	91.20	E
MOTA	8841	C	LYS E	199	79.7	14 32	.154 63	9.545	1.00	75.13	E
MOTA	8842	0	LYS E	199	80.3	40 32	.744 68	8.672	1.00	76.16	E
MOTA	8843	N	MET E	200	80.2	50 31	.180 70	0.268	1.00	76.95	E
ATOM	8844	CA	MET E	200	81.6	20 30		0.031	1.00	78.07	E
MOTA	8845	CB	MET E	200	82.5	31	.087 73	1.222	1.00	80.58	E
ATOM	8846	CG	MET E	200	81.9	02 32	.082 73	2.179	1.00	83.33	E
MOTA	8847	SD	MET B		83.1	.57 32	.884 73	3.180	1.00	94.18	E
ATOM	8848	CE	MET E		82.6	35 34	.607 73	3.015	1.00	92.27	E
MOTA	8849	C	MET B		81.6	10 29	.244 69	9.806	1.00	77.40	E
ATOM	8850	0	MET E	200	80.6	27 28	.573 70	0.135	1.00	76.60	E
MOTA	8851	N	THR E		82.7	03 28	.720 69	9.254	1.00	77.22	E
ATOM	8852	CA	THR B		82.7	98 27	.293 68	3.967	1.00	77.48	E
MOTA	8853	CB	THR E		83,-5	00 27	.038 67	7.611	1.00	76.20	E
MOTA	· 8854	OG1	THR E		82.7	48 27	.660 66	5.560	1.00	76.69	E
MOTA	8855	CG2	THR E	201	83.5	91 25	.542 67	7.332	1.00	71.96	E
MOTA	8856	C	THR E		83.5		.480 70	0.037	1.00	77.79	E
MOTA	8857	0	THR E		84.5	82 26	.855 70).517	1.00	78.02	E
ATOM	8858	И	GLY E		82.9	00 25	.356 70	394	1.00	78.70	E
MOTA	8859	CA	GLY E		83.4	70 24	.476 7]	1.392	1.00	83.61	E
ATOM	8860	С	GLY E		84.8	76 24	.068 71	L.016	1.00	86.50	E
MOTA	8861	0	GLY E		85.1		.706 69	868	1.00	87.22	E
MOTA	8862	N	VAL E		85.7			L.988	1.00	88.73	E
ATOM	8863	CA	VAL E		87.1			1.764		91.05	E
MOTA	8864	CB	VAL E		88.0			L.845		90.32	E
MOTA	`8865		VAL E		89.4			L.492		87.74	E
MOTA	8866		VAL E		87.4			920		85.78	E
ATOM	8867	C	VAL E	_	87.6			2.796		93.95	E
ATOM	8868	0	VAL E		88.4			3.714		96.85	E
MOTA	8869	N	MET E		87.2			2.638		95.46	E
MOTA	8870	CA	MET E		87.6			3.566		98.14	E
ATOM	8871	CB	MET E		87.3			2.948		01.59	E
ATOM	8872	CG	MET E		85.8			2.658		05.16	E
MOTA	8873	SD	MET E		85.1			L.448		12.63	E
MOTA	8874	CE	MET E		85.5			897		10.01	E
ATOM	8875	C	MET E		89.1			3.982		97.01	E
ATOM	8876	0	MET E		90.0			3.148		95.27	E
MOTA	8877	N	GLU E		89.3			5.280		99.01	E
ATOM	8.878	CA	GLU E		90.7			5.780	1.001		E
MOTA	8879	CB	GLU E		90.8			7.218		05.77	E
MOTA	8880	CG	GLU E		90.2			3.275		12.16	E
ATOM	8881	CD	GLU E		91.2			3.407	1.001		E
MOTA	8882		GLU E		90.9			345	1.001		B
MOTA	8883	OE2	GLU E	205	92.3	85 20	.313 79	3.356	1.001	16.20	В

MOTA	8884	С	GLU	E	205		91.305	19.012	75.746	1.00104.46	E
ATOM	8885	0	GLU	E	205		92.488	18.867	75.373	1.00104.28	E
MOTA	8886	OXT	GLU	E	205		90.553	18.079	76.112	1.00107.35	E
MOTA	8887	CB	PHE	F	1		80.812	82.422	60.648	1.00 33.92	F
MOTA	8888	CG	PHE	F	1		80.164	81.444	61.587	1.00 35.95	F
MOTA	8889	CD1	PHE	F	1		79.979	80.113	61.215	1.00 39.29	F
ATOM	8890	CD2	PHE	F	1		79.786	81.834	62.867	1.00 34.66	F
MOTA	8891	CEL	PHE	F	1		79.436	79.192	62.102	1.00 30.20	F
MOTA	8892	CE2	PHE		1		79.238	80.916	63.765	1.00 30.16	· F
MOTA	8893	CZ	PHE		1		79.066	79.595	63.380		F
MOTA	8894	C	PHE		1		82.921	81.051	60.380	1.00 30.85	F
ATOM	8895	Ó	PHE		1		82.798	80.576	59.260	1.00 28.03	F
ATOM	8896	N	PHE		1		82.903	83.402	59.737	1.00 39.15	F
ATOM	8897	CA	PHE		1		82.354	82.424	60.714	1.00 34.90	F
ATOM	8898	N	ALA		2		83.561	80.428	61.359	1.00 32.93	F
ATOM	8899	CA	ALA		2		84.156	79.107	61.178	1.00 32.00	F
MOTA	8900	CB.	ALA		2		85.591	79.252	60.743	1.00 22.11	F
ATOM	8901	C	ALA		2		84.083	78.330	62.492	1.00 32.49	F
ATOM	8902	ō	ALA		2		83.977	78.919	63.574	1.00 33.00	F
ATOM	8903	N	CYS		3		84.141	77.007	62.408	1.00 30.62	F
ATOM	8904	CA	CYS		3		84.078	76.196	63.615	1.00 31.66	F
ATOM	8905	C	CYS		3		85.190	75.150	63.624	1.00 31.86	F
ATOM	8906	ŏ	CYS		3		85.765	74.840	62.590	1.00 31.93	F
ATOM	8907	CB	CYS		3		82.730	75.497	63.709	1.00 32.29	ŕ
ATOM	8908	SG	CYS		3		81.240	76.539	63.584	1.00 40.59	F
ATOM	8909	N	LYS		4		85.503	74.619	64.799	1.00 32.55	F
ATOM	8910	CA	LYS		4		86.533	73.603	64.916	1.00 35.01	F
ATOM	8911	CB	LYS		4		87.888	74.203	65.308	1.00 34.04	
ATOM	8912	CG	LYS		4		87.932	74.783	66.712	1.00 34.04	F F
ATOM	8913	CD .	LYS		4		89.251	75.509	67.023	1.00 43.55	F
ATOM	8914	CE	LYS		4		90.432	74.554	67.175	1.00 53.56	F
ATOM	8915	NZ	LYS		4		90.788	73.874	65.896	1.00 70.19	r T
ATOM	8916	C	LYS		4		86.127	72.577	65.958	1.00 70.19	F
ATOM	8917	o	LYS		4		85.294	72.817	66.831		
ATOM	8918	N	THR		5		86.764	71.427		1.00 39.09	F
ATOM	8919	CA	THR		5		86.507	70.316	65.854	1.00 40.82	F
ATOM	8920	CB	THR		5		86.375	69.051	66.717 65.844	1.00 36.59	F
ATOM	8921	OG1	THR		5		85.177		66.198	1.00 34.26	F
ATOM	8922	CG2	THR		5		87.547	68.363 68.157		1.00 41.95	F
ATOM	8923	C	THR		5		87.627	70.240	65.979 67.730	1.00 26.04	P
ATOM	8924	ŏ	THR		5		88.792	70.435	67.401	1.00 35.59	F F
ATOM	8925	N	ALA		6		87.254			1.00 38.72 1.00 36.62	
ATOM	8926	CA	ALA		. 6		88.208	69.996	68.979	_	F
ATOM	8927	CB	ALA		. 6		87.492	69.912 69.541	70.076 71.354	1.00 34.75	F
ATOM	8928	C	ALA		6		89.282		69.773	1.00 32.49	F F
ATOM	8929	ō	ALA		6		90.390	68.902 68.975	70.291	1.00 36.90	F
ATOM	8930	N	ASN		7			67.953		1.00 37.23	_
ATOM	8931	CA	ASN		7		88.948		68.916	1.00 45.57	F
ATOM	8932	CB	ASN		7		89.887	66.904	68.537	1.00 49.55	F
ATOM	8933	CG	ASN	r r	7		89.151 89.688	65.768	67.845	1.00 51.09	F
ATOM	8934		ASN					64.422	68.235	1.00 57.54	F
MOTA					7		90.699	64.329	68.943	1.00 59.53	F
	8935		ASN		7		89.019	63.362	67.783	1.00 49.46	F
ATOM ATOM	8936	C	ASN		7		90.940	67.449	67.608	1.00 48.81	F
	8937	0 N	ASN		7		92.106	67.046	67.666	1.00 53.22	F
ATOM	8938	N	GLY		8		90.508	68.363	66.750	1.00 47.63	된
ATOM	8939	CA	GLY		8		91.406	68.988	65.806	1.00 53.31	F
ATOM	8940	C	GLY	F	8		90.738	69.585	64.568	1.00 57.85	F
ATOM	8941	0	GLY	r	8	:	90.991	70.750	64.226	1.00 59.56	F

MOTA	8942	N	THR	F.	9	89.876	68.801	63.910	1.00 53.29	F
MOTA	8943	CA	THR	F	9	89.202	69.206	62.672	1.00 49.01	F
MOTA	8944	CB	THR	F	9	88.340	68.067	62.160	1.00 51.01	F
MOTA	8945	OG1	THR	F	9	89.162	66.901	62.022	1.00 63.11	F
MOTA	8946	CG2	THR	F	9	87.738	68.415	60.810	1.00 47.64	F
MOTA	8947	C	THR		9	88.379	70.489	62.629	1.00 47.40	F
MOTA	8948	0	THR		9	87.712	70.854	63.588	1.00 49.35	F
ATOM	8949	N	ALA	F	10	88.423	71.154	61.474	1.00 44.85	F
ATOM	8950	CA	ALA		10	87.717	72.415	61.249	1.00 38.12	F
ATOM	8951	CB	ALA		10	88.721	73.552	61.113	1.00 27.66	F
MOTA	8952	C	ALA		10	86.840	72.408	60.017	1.00 36.08	F
ATOM	8953	0	ALA		10	87.027	71.606	59.105	1.00 39.20	F
ATOM	8954	N	ILE		11	85.869	73.311	60.008	1.00 31.43	F
ATOM	8955	CA	ILE		11	85.001	73.485	58.860	1.00 32.87	F
ATOM	8956	CB	ILE		11	83.554	73.186	59.172	1.00 34.87	F
ATOM	8957	CG2	ILE		11	82.728	73.391	57.916	1.00 35.36	F
ATOM	8958	CG1	ILE		11	83.421	71.755	59.699	1.00 37.73	F
ATOM ATOM	8959	CD1			11	82.010	71.357	60.058	1.00 34.84	F
ATOM	8960	C	ILE		11	85.160	74.965	58.625	1.00 33.05	F
ATOM	8961 8962	И О	ILE PRO		11 12	84.819 85.680	75.771 75.347	59.476	1.00 40.18	F
ATOM	8963	CD	PRO		12	86.123	74.482	57.468 56.362	1.00 29.45	F F
ATOM	8964	CA	PRO		12	85.898	76.753	57.147	1.00 31.75 1.00 31.33	
ATOM	8965	CB	PRO		12	86.914	76.670	56.018	1.00 35.39	F F
ATOM	8966	CG	PRO		12	86.406	75.486	55.244	1.00 33.33	F
ATOM	8967	C	PRO		12	84.696	77.592	56.752	1.00 32.23	F
ATOM	8968	ō	PRO		12	83.570	77.093	56.661	1.00 31.88	F
ATOM	8969	N	ILE		13	84.983	78.878	56.520	1.00 31.86	F
ATOM	8970	CA	ILE		13	84.017	79.885	56.073	1.00 31.16	·F
MOTA	8971	CB	ILE		13	84.750	81.185	55.638	1.00 32.37	F
MOTA	8972	CG2	'ILE	F	13	83.809	82.104	54.849	1.00 31.26	F
MOTA	8973	CG1	ILE	F	13	85.328	81.882	56.873	1.00 32.40	F
MOTA	8974	CD1	ILE	F	13	86.079	83.116	56.569	1.00 26.26	F
MOTA	8975	С	ILE	F	13	83.304	79.310	54.864	1.00 29.77	F
MOTA	8976	0	ILE		13	83.961	78.796	53.969	1.00 31.36	F
ATOM	8977	Ν.	GLY	F	14	81.976	79.387	54.838	1.00 27.74	F
ATOM	8978	CA	GLY		14	81.228	78.849	53.714	1.00 28.67	F
MOTA	8979	С	GLY		14	80.606	77.490	54.011	1.00 33.28	F
MOTA	8980	0	GLY		14	79.811	76.961	53.223	1.00 34.40	F
MOTA	8981	N	GLY		15	80.982	76.902	55.141	1.00 33.08	F
ATOM	8982	CA	GLY		15	80.407	75.622	55.517	1.00 30.57	F
ATOM	8983	C	GLY		15	81.160	74.389	55.063	1.00 31.84	F
ATOM	8984	0	GLY		15	82.195	74.473	54.401	1.00 34.18	F
ATOM ATOM	8985 8986	N CA	GLY GLY		16	80.614	73.232	55.422	1.00 27.95	F
ATOM	8987	CA			16	81.226	71.966	55.087	1.00 20.25	F
	8988	0	GLY		16 16	80.855 79.848	70.962 71.114	56.155 56.836	1.00 20.58 1.00 26.27	F
ATOM	8989	N	SER		17	81.666	69.941	56.354	1.00 26.27	F F
ATOM	8990	CA	SER		17	81.298	68.954	57.343	1.00 16.79	F
ATOM	8991	CB	SER		17	80.490	67.847	56.665	1.00 16.79	
ATOM	8992	OG	SER		17	81.331	66.996	55.896	1.00 22.29	F F
ATOM	8993	C	SER		17	82.473	68.343	58.060	1.00 27.14	F
ATOM	8994	ō	SER		17	83.583	68.326	57.541	1.00 18.53	F
ATOM	8995	N	ALA		18	82.230	67.822	59.257	1.00 13.27	F
ATOM	8996	CA	ALA		18	83.302	67.191	60.020	1.00 15.38	F
ATOM	8997	CB	ALA		18	84.042	68.213	60.837	1.00 10.31	F
MOTA	8998	C	ALA		18	82.787	66.119	60.930	1.00 21.83	F
ATOM	8999	ō	ALA		18	81.616	66.105	61.300	1.00 31.45	F
										-

MOTA	9000	N	ASN	F	19	83.685	65.222	61.301	1.00 22.39	F
MOTA	9001	CA	ASN	F	19	83.368	64.129	62.202	1.00 21.13	F
MOTA	9002	CB	ASN		19	84.265	62.916	61.930	1.00 19.51	F
MOTA	9003	CG	ASN		19	83.837	62.124	60.708	1.00 19.53	F
ATOM	9004		ASN		19	82.875	62.470	60.029	1.00 15.43	F
ATOM	9005		ASN		19	84.564	61.052	60.421	1.00 13.23	F
MOTA	9006	C	ASN		19	83.636	64.572	63.621	1.00 24.69	F
ATOM	9007	0	ASN		19	84.599	65.278	63.889	1.00 26.24	F
ATOM	9008	N	VAL		20	82.792	64.145	64.541	1.00 27.12	F
MOTA	9009	CA	VAL		20	83.017	64.459	65.936	1.00 27.32	F
ATOM	9010	CB	VAL		20	81.945 82.293	65.391	66.451	1.00 28.40	F
ATOM ATOM	9011 9012		VAL VAL		20 20	81.849	65.810 66.602	67.861	1.00 30.24 1.00 18.25	F
MOTA	9012	C	VAL		20	82.999	63.129	65.528 66.690	1.00 16.25	F
ATOM	9014	ō	VAL		20	81.965	62.473	66.774	1.00 28.82	F F
ATOM	9015	N	TYR		21	84.151	62.726	67.213	1.00 23.34	F
ATOM	9016	CA	TYR		21	84.279	61.454	67.940	1.00 26.68	F
ATOM	9017	CB	TYR		21	85.650	60.844	67.653	1.00 19.01	F
ATOM	9018	CG	TYR		21	85.959	60.791	66.182	1.00 28.25	F
ATOM	9019		TYR		21	86.786	61.740	65.592	1.00 24.71	F
ATOM	9020	CE1			21	87.030	61.723	64.214	1.00 31.01	F
MOTA	9021	CD2	TYR	F	21	85.379	59.814	65.359	1.00 25.81	F
ATOM	9022	CE2	TYR	F	21	85.618	59.787	63.988	1.00 29.45	F
ATOM	9023	CZ	TYR	F	21	86.447	60.744	63.422	1.00 34.73	F
MOTA	9024	OH.	TYR	F	21	86.723	60.710	62.078	1.00 35.46	F
MOTA	9025	C	TYR	F	21	84.069	61.562	69.455	1.00 29.69	F
MOTA	9026	0	TYR		21	84.840	62.230	70.155	1.00 33.08	F
MOTA	9027	N	VAL		22	83.048	60.869	69.963	1.00 31.10	F
MOTA	9028	CA	VAL		22	82.704	60.925	71.390	1.00 30.65	F
MOTA	9029	CB	VAL		22	81.277	61.440	71.602	1.00 25.94	F
ATOM	9030		VAL		22	81.109	62.803	70.978	1.00 23.02	F
MOTA	9031		VAL		22	80.299	60.455	71.013	1.00 24.67	F
MOTA	9032	C	VAL		22	82.772	59.646	72.202	1.00 31.76	F
ATOM	9033	0	VAL		22	82.265	58.607	71.773	1.00 30.44	F
ATOM	9034	N	asn Asn		23 23	83.371	59.740	73.391	1.00 32.82	F
ATOM ATOM	9035 9036	CA CB	ASN		23	83.441	58.607	74.308	1.00 32.03	F
ATOM	9037	CG	ASN		23	84.661 85.867	58.721 59.131	75.179 74.410	1.00 32.85 1.00 34.07	F F
ATOM	9038		ASN		23	86.613	58.303	73.879	1.00 34.83	F
ATOM	9039		ASN		23	86.068	60.431	74.326	1.00 43.60	F
ATOM	9040	c	ASN		23	82.195	58.748	75.183	1.00 31.34	F
ATOM	9041	ō	ASN		23	82.003	59.786	75.803	1.00 29.30	F
ATOM	9042	N	LEU		24	81.353	57.721	75.222	1.00 31.60	F
ATOM	9043	CA	LEU	F	24	80.114	57.766	76.009	1.00 32.96	F
MOTA	9044	CB	LEU	F	24	78.938	57.325	75.129	1.00 29.44	F
ATOM	9045	CG	LEU	F	24	78.785	57.994	73.764	1.00 25.79	F
ATOM	9046	CD1	LEU	F	24	78.076	57.049	72.820	1.00 22.87	F
MOTA	9047	CD2	LEU	F	24	78.018	59.293	73.886	1.00 28.59	F
ATOM	9048	C	LEU	F	24	80.143	56.869	77.256	1.00 33.03	F
MOTA	9049	0	LEU		24	80.927	55.925	77.324	1.00 36.91	F
ATOM	9050	N	ALA		25	79.290	57.166	78.236	1.00 29.98	F
ATOM	9051	CA	ALA	F	25	79:184	56.338	79.446	1.00 29.57	F
ATOM	9052	CB	ALA		25	77.962	56.726	80.201	1.00 25.78	F
MOTA	9053	C	ALA		25	79.051	54.891	78.974	1.00 32.98	F
ATOM	9054	0	ALA		25	78.171	54.573	78.192	1.00 39.53	F
ATOM ·	9055	И	PRO		26	79.900	53.992	79.455	1.00 31.64	F
ATOM	9056	CD	PRO		26	80.913	54.190	80.491	1.00 34.85	F
MOTA	9057	CA	PRO	F	26	79.856	52.584	79.039	1.00 33.70	F

MOTA	9058	CB	PRO	F	26	81.065	51.963	79.765	1.00 35.76	F
ATOM	9059	CG	PRO	F	26	81.916	53.110	80.123	1.00 41.95	F
MOTA	9060	C	PRO	F	26	78.570	51.802	79.343	1.00 35.04	F
ATOM	9061	0	PRO	F	26	78.246	50.830	78.654	1.00 30.95	F
ATOM	9062	N	VAL	F	27	77.862	52.226	80.386	1.00 35.37	F
MOTA	9063	CA	VAL	F	27	76.642	51.575	80.840	1.00 31.59	F
MOTA	9064	CB	VAL	F	27	76.906	50.790	82.128	1.00 34.64	F
ATOM	9065	CG1	VAL	F	27	75.607	50.240	82.691	1.00 35.51	F
ATOM	9066	CG2	VAL	F	27	77.907	49.697	81.865	1.00 33.14	F
MOTA	9067	C	VAL	F	27	75.562	52.583	81.161	1.00 31.10	F
MOTA	9068	0	VAL	F	27	75.809	53.593	81.802	1.00 34.90	F
MOTA	9069	N	VAL	F	28	74.348	52.290	80.745	1.00 32.54	F
ATOM	9070	CA	VAL	F	28	73.227	53.177	81.012	1.00 34.96	F
ATOM	9071	CB	VAL	F	28	72.965	54.118	79.808	1.00 31.97	F
ATOM	9072	CG1	VAL	F	28	71.854	55.105	80.119	1.00 34.44	F
MOTA	9073	CG2	VAL		28	74.230	54.851	79.459	1.00 30.03	F
MOTA	9074	C	VAL	F	28	72.036	52.248	81.234	1.00 40.51	F
MOTA	9075	0	VAL	F	28	71.858	51.255	80.513	1.00 42.64	F
MOTA	9076	N	ASN		29	71.226	52.553	82.240	1.00 41.21	F
ATOM	9077	CA	ASN	F	29	70.081	51.705	82.538	1.00 40.01	F
MOTA	9078	CB	asn	F	29	69.848	51.600	84.043	1.00 33.89	F
MOTA	9079	CG	ASN	F	29	71.058	51.096	84.780	1.00 39.67	F
MOTA	9080		ASN		29	71.560	50.014	84.496	1.00 43.68	F
MOTA	9081		ASN		29	71.539	51.879	85.743	1.00 47.58	F
MOTA	9082	C	ASN		29	68.831	52.244	81.924	1.00 38.61	F
MOTA	9083	0	ASN		29	68.730	53.443	81.643	1.00 34.33	F
MOTA	9084	N	VAL		30	67.867	51.350	81.736	1.00 36.25	F
MOTA	9085	CA	VAL		30	66.590	51.758	81.199	1.00 38.11	F
ATOM	9086	CB.	VAL		30	65.587	50.599	81.221	1.00 36.54	F
ATOM	9087		VAL		30	64.214	51.075	80.744	1.00 31.95	F
MOTA	9088		VAL		30	66.094	49.466	80.337	1.00 31.08	F
MOTA	9089	, C	VAL		30	66.147	52.841	82.166	1.00 41.13	F
ATOM	9090	0	VAL		30	66.435	52.751	83.355	1.00 42.21	F
MOTA	9091	N	GLY		31	65.497	53.882	81.661	1.00 45.46	F
MOTA	9092	CA	GLY		31	65.038	54.941	82.542	1.00 50.57	F
MOTA	9093	C	GLY		31	66.019	56.082	82.739	1.00 54.66	F
ATOM	9094	0	GLY		31	65.601	57.218	82.947	1.00 57.31	F
MOTA	9095	N	GLN		32	67.317	55.795	82.674	1.00 54.51	F
MOTA	9096	.CA	GLN		32	68.337	56.826	82.845	1.00 53.70	P
ATOM	9097	CB	GLN		32	69.630	56.188	83.342	1.00 54.96	F
ATOM	9098	CG	GLN		32	69.729	56.091	84.847	1.00 66.08	F
MOTA	9099	CD		F	32	70.815	55.124	85.296	1.00 73.26	F
ATOM	9100		GLN		32	71.911	55.085	84.720	1.00 71.06	F
MOTA	9101	NE2	GLN		32	70.518	54.339	86.340	1.00 75.66	F
MOTA	9102	C	GLN		32	68.627	57.656	81.583	1.00 53.14	F
ATOM	9103	0	GLN		32	68.056	57.430	80.516	1.00 51.96	F
ATOM	9104	N	ASN		33	69.518	58.630	81.729	1.00 51.12	F
ATOM	9105 9106	CA	ASN		33	69.908	59.502	80.630	1.00 47.87	F
ATOM		CB	ASN		33	69.747	60.968	81.024	1.00 42.01	F
ATOM	9107	CG	ASN ASN		33	68.438	61.561	80.553	1.00 45.78	F
ATOM	9108				33	68.066	62.669	80.951	1.00 38.33	F
ATOM ATOM	9109 9110	C MD2	ASN ASN		33	67.735	60.837	79.689	1.00 43.12	F
	9110	0			33	71.347	59.299	80.187	1.00 48.45	F
ATOM ATOM		И	ASN LEU		33	72.271	59.220	80.996	1.00 48.59	F
ATOM	9112 9113	CA	LEU		34	71.527	59.186	78.885	1.00 50.50	F
ATOM	9113	CB	LEU		34	72.856	59.079	78.314	1.00 48.19	F
ATOM	9114	CG	LEU		34	72.873	58.110	77.142	1.00 48.47	F
WT OM	フエエコ	CG	ngu	£	34	74.152	58.169	76.321	1.00 45.89	F

MOTA	9116	CD1	LEU	F	34	75.297	57.484	77.046	1.00 42.48	F
MOTA	9117	CD2	LEU	F	34	73.874	57.510	74.990	1.00 49.15	· F
MOTA	9118	C	LEU	F	34	73.013	60.509	77.812	1.00 47.21	F
MOTA	9119	0	LEU	F	34	72.134	61.041	77.113	1.00 43.62	F
MOTA	9120	N	VAL	F	35	74.108	61.150	78.183	1.00 43.20	F
MOTA	9121	CA	VAL	F	35	74.284	62.519	77.764	1.00 41.46	F
ATOM	9122	CB	VAL	F	35	74.430	63.441	78.984	1.00 41.50	F
ATOM	9123	CG1	VAL	F	35	74.542	64.883	78.538	1.00 38.83	F
ATOM	9124	CG2	VAL	F	35	73.232	63.260	79.892	1.00 37.25	F
MOTA	9125	C	VAL	F	35	75.467	62.712	76.851	1.00 37.06	F
MOTA	9126	0	VAL	F	35	76.590	62.344	77.194	1.00 37.06	F
MOTA	9127	N	VAL	F	36	75.201	63.277	75.677	1.00 34.47	F
MOTA	9128	CA	VAL	F	36	76.265	63.553	74.725	1.00 36.32	F
MOTA	9129	CB	VAL	F	36	75.959	63.024	73.328	1.00 38.02	F
MOTA	9130	CG1	VAL	F	36	77.263	62.774	72.612	1.00 41.12	F
ATOM	9131	CG2	VAL	F	36	75.146	61.757	73.409	1.00 37.10	F
MOTA	9132	C	VAL	F	36	76.336	65.047	74.654	1.00 34.58	F
MOTA	9133	0	VAL	F	36	75.472	65.691	74.054	1.00 34.73	F
MOTA	9134	N	ASP		37	77.356	65.610	75.284	1.00 36.96	F
MOTA	9135	CA	ASP	F	37	77.495	67.061	75.296	1.00 43.47	F
MOTA	9136	CB	ASP	F	37	77.906	67.525	76.693	1.00 46.50	·F
MOTA	9137	CG	ASP	F	37	77.849	69.028	76.845	1.00 55.92	F
ATOM	9138		ASP		37	76.826	69.633	76.431	1.00 59.16	F
ATOM	9139	OD2	ASP	F	37	78.826	69.599	77.386	1.00 58.57	F
ATOM	9140	C	ASP	F	37	78.498	67.544	74.258	1.00 40.22	F
MOTA	9141	0	ASP		37	79.708	67.411	74.442	1.00 41.05	F
MOTA	9142	N	LEU	F	38	77.992	68.118	73.175	1.00 37.20	F
MOTA	9143	CA	LEU	F	38	78.870	68.579	72.112	1.00 39.70	F
MOTA	9144	CB	LEU	F	38	78.125	68.526	70.783	1.00 36.96	. F
MOTA	9145	CG	LEU		38	77.812	67.057	70.508	1.00 30.31	F
MOTA	9146	CD1			38	76.853	66.949	69.386	1.00 44.81	F
MOTA	9147	CD2			38 ୍	79.077	66.305	70.179	1.00 34.21	F
MOTA	9148	C	LEU		38	79.490	69.945	72.340	1.00 39.97	F
MOTA	9149	0	LEU		38	80.518	70.271	71.726	1.00 34.44	F
MOTA	9150	N	SER		39	78.868	70.719	73.234	1.00 42.07	F
MOTA	9151	CA	SER		39	79.330	72.059	73.608	1.00 39.92	F
MOTA	9152	CB	SER		39	78.472	72.639	74.725	1.00 43.81	F
ATOM	9153	OG	SER		39	78.915	72.141	75.981	1.00 39.88	F
ATOM	9154	C	SER		39	80.730	71.893	74.158	1.00 35.42	F
ATOM	9155	0	SER		39	81.441	72.853	74.403	1.00 38.86	F
MOTA	9156	N	THR		40	81.114	70.656	74.381	1.00 31.46	· F
ATOM	9157	CA	THR		40	82.429	70.398	74.890	1.00 30.14	F
ATOM	9158	CB	THR		40	82.368	69.253	75.910	1.00 28.16	F
ATOM	9159	OG1	THR		40	82.804	69.753	77.172	1.00 36.75	F
ATOM	9160	CG2	THR		40	83.241	68.079	75.503	1.00 23.29	F
ATOM	9161	C	THR		40	83.350	70.042		1.00 31.05	F
ATOM	9162	0	THR		40	84.572	70.011	73.892	1.00 28.36	F
ATOM	9163	N	GLN		41	82.765	69.789	72.571	1.00 33.63	F
MOTA MOTA	9164	CA	GLN GLN		41	83.573	69.382	71.432	1.00 36.47	F
ATOM	9165	CB			41	83.286	67.922	71.121	1.00 40.54	F
	9166	CG	GLN		41	83.720	66.995	72.226	1.00 40.60	F
ATOM	9167	CD	GLN		41	84.377	65.774	71.673	1.00 48.50	F
MOTA MOTA	9168	NE2	GLN GLN		41	83.710	64.857	71.182	1.00 50.59	F
ATOM	9169	C NEZ	GLN		41	85.704	65.754	71.714	1.00 55.45	F
ATOM	9170 9171		GLN		41	83.460	70.193	70.152	1.00 36.38	F
ATOM	9171	и О	ILE		41	84.242	69.984	69.223	1.00 32.40	F
ATOM	9172 9173	CA	ILE		42	82.499	71.112	70.098	1.00 34.19	F
WION	21/3	CH.	TTIC	£	42	82.320	71.928	68.908	1.00 33.92	F

ATOM 9174 CB ILE F 42 88.0872 71.550 68.200 1.00 29.76 F ATOM 9175 CG2 ILE F 42 88.0872 72.358 66.935 1.00 33.58 F ATOM 9177 CD1 ILE F 42 88.0872 72.358 66.935 1.00 33.58 F ATOM 9177 CD1 ILE F 42 82.316 73.425 69.224 1.00 37.57 F ATOM 9179 CD ILE F 42 82.316 73.425 69.224 1.00 37.57 F ATOM 9180 N PHE F 43 83.437 75.571 68.823 1.00 34.58 F ATOM 9180 N PHE F 43 83.439 75.571 68.823 1.00 39.76 F ATOM 9181 CD PHE F 43 84.480 75.586 69.224 1.00 39.76 F ATOM 9181 CD PHE F 43 84.480 75.586 69.224 1.00 39.75 F ATOM 9182 CD PHE F 43 84.480 75.158 70.836 1.00 39.75 F ATOM 9185 CD PHE F 43 84.480 75.158 70.836 1.00 39.75 F ATOM 9185 CD PHE F 43 84.480 75.158 70.836 1.00 38.48 F ATOM 9185 CD PHE F 43 84.480 75.158 70.836 1.00 38.48 F ATOM 9185 CD PHE F 43 84.491 75.803 72.013 1.00 41.38 F ATOM 9186 CE PHE F 43 84.491 75.803 72.013 1.00 40.49 F ATOM 9187 CD PHE F 43 84.491 75.803 72.013 1.00 40.49 F ATOM 9189 C PHE F 43 84.491 75.803 72.013 1.00 40.49 F ATOM 9189 C PHE F 43 84.997 73.818 73.300 1.00 39.96 F ATOM 9189 C PHE F 43 84.997 73.818 73.300 1.00 39.543 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9190 C PHE F 43 83.997 76.404 67.561 1.00 39.77 F ATOM 9190 C PHE F 43 83.997 76.404 67.561 1.00 39.77 F ATOM 9190 C PHE F 43 83.997 76.404 67.561 1.00 39.78 F ATOM 9191 N CYS F 44 82.724 78.492 66.535 1.00 39.88 F ATOM 9192 CA CYS F 44 83.291 80.893 79.894 66.573 1.00 40.453 F ATOM 9195 C C CYS F 44 83.291 80.200 68.163 1.00 40.53 F ATOM 9195 C C CYS F 44 83.291 80.200 68.163 1.00 40.53 F ATOM 9195 C C CYS F 44 83.291 80.200 68.163 1.00 40.53 F ATOM 9195 C C CYS F 44 83.291 80.200 68.163 1.00 40.53 F ATOM 9195 C C C C C C C C C C C C C C C C C C C											
ATOM 9176 CGI ILE F 42 81.040 70.062 67.872 1.00 31.94 F ATOM 9177 CDI ILE F 42 79.741 69.572 67.315 1.00 32.41 F ATOM 9179 O ILE F 42 82.316 73.425 69.224 1.00 37.57 F ATOM 9180 N PHE F 43 83.475 74.133 68.625 1.00 40.15 F ATOM 9180 N PHE F 43 83.439 75.571 68.823 1.00 39.76 F ATOM 9181 CA PHE F 43 84.839 75.571 68.823 1.00 39.76 F ATOM 9181 CA PHE F 43 84.859 75.846 69.528 1.00 37.57 F ATOM 9181 CA PHE F 43 84.880 75.158 70.836 1.00 38.48 F ATOM 9185 CD PHE F 43 84.880 75.158 70.836 1.00 38.48 F ATOM 9185 CD PHE F 43 84.880 73.158 70.836 1.00 38.48 F ATOM 9185 CD PHE F 43 84.891 73.803 72.013 1.00 40.49 F ATOM 9185 CD PHE F 43 84.891 73.803 73.614 10.00 40.49 F ATOM 9186 CE PHE F 43 84.491 75.803 72.013 1.00 40.63 F ATOM 9187 CE2 PHE F 43 84.491 75.803 72.013 1.00 40.63 F ATOM 9187 CE2 PHE F 43 84.97 73.818 73.200 1.00 39.77 F ATOM 9189 C PHE F 43 84.97 73.818 73.200 1.00 39.77 F ATOM 9189 C PHE F 43 84.97 73.818 73.200 1.00 39.77 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9190 O PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9191 N CYS F 44 82.796 77.581 66.593 1.00 39.77 F ATOM 9191 N CYS F 44 82.796 77.581 66.973 1.00 39.84 F ATOM 9193 C CYS F 44 82.724 78.492 66.535 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.84 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.94 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 39.94 F ATOM 9195 CB CYS F 44 83.115 79.913 66	MOTA	9174	CB	ILE	F	42	81.025	71.550	68.200	1.00 29.76	F
ATOM 9177 CD1 ILE F 42 79.741 69.572 67.315 1.00 32.41 F ATOM 9178 C ILE F 42 82.316 73.425 69.224 1.00 37.57 F ATOM 9180 N PHB F 43 83.439 75.571 68.623 1.00 33.58 F ATOM 9181 CA PHE F 43 83.439 75.571 68.623 1.00 33.75 F ATOM 9182 CB PHE F 43 84.757 75.846 69.528 1.00 33.75 F ATOM 9182 CB PHE F 43 84.850 75.158 70.836 1.00 33.75 F ATOM 9183 CG PHE F 43 84.850 75.158 70.836 1.00 33.75 F ATOM 9184 CD1 PHE F 43 85.320 73.841 70.990 1.00 38.96 F ATOM 9185 CD2 PHE F 43 85.330 73.841 70.990 1.00 38.96 F ATOM 9185 CD2 PHE F 43 85.330 73.841 70.990 1.00 38.96 F ATOM 9185 CD2 PHE F 43 84.891 75.893 72.013 1.00 44.49 F ATOM 9186 CE1 PHE F 43 84.537 73.644 72.123 1.00 40.49 F ATOM 9187 CE2 PHE F 43 84.537 73.642 72.013 1.00 40.49 F ATOM 9187 CE2 PHE F 43 84.537 73.618 73.300 1.00 35.43 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9190 O PHE F 43 83.395 76.000 66.520 1.00 42.10 F ATOM 9191 N CYS F 44 82.724 78.492 66.535 1.00 40.63 F ATOM 9191 N CYS F 44 82.724 78.492 66.535 1.00 40.53 F ATOM 9191 C CYS F 44 83.271 80.200 68.6163 1.00 40.53 F ATOM 9195 CB CYS F 44 83.215 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.215 79.913 66.973 1.00 40.53 F ATOM 9195 CG CYS F 44 83.215 80.200 68.6163 1.00 41.55 F ATOM 9195 CG CYS F 44 83.271 80.200 68.6163 1.00 41.55 F ATOM 9195 CG CYS F 44 83.271 80.200 68.6163 1.00 41.55 F ATOM 9195 CG CYS F 44 83.271 80.200 68.6163 1.00 41.55 F ATOM 9195 CG CYS F 44 83.271 80.200 68.6163 1.00 41.55 F ATOM 9195 CG CYS F 44 83.271 80.200 68.6163 1.00 41.55 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.76 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.76 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.76 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.76 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.71 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.71 F ATOM 9195 CG CYS F 45 83.295 80.801 66.005 1.00 38.71 F ATOM 9195 CG CYS F 45 83	MOTA	9175	CG2	ILE	F	42	80.872	72.358	66.935	1.00 33.58	F
ATOM 9178 C ILE F 42 81.462 73.920 69.921 1.00 37.57 F ATOM 9179 O ILE F 42 81.462 73.920 69.981 1.00 34.58 F ATOM 9180 N PHE F 43 83.476 74.333 68.625 1.00 40.15 F ATOM 9181 CA PHE F 43 83.476 74.333 68.625 1.00 37.57 F ATOM 9181 CA PHE F 43 84.839 75.571 68.823 1.00 39.76 F ATOM 9182 CB PHE F 43 84.880 75.158 70.836 1.00 38.48 F ATOM 9183 CG PHE F 43 84.880 73.481 70.990 1.00 39.96 F ATOM 9185 CD2 PHE F 43 84.880 73.481 70.990 1.00 39.96 F ATOM 9185 CD2 PHE F 43 84.891 73.803 72.013 1.00 41.38 F ATOM 9185 CD2 PHE F 43 84.891 73.803 72.013 1.00 41.38 F ATOM 9186 CE2 PHE F 43 84.919 73.818 73.300 1.00 41.38 F ATOM 9187 CE2 PHE F 43 84.919 73.818 73.300 1.00 42.00 39.97 F ATOM 9180 C PHE F 43 84.919 73.818 73.300 1.00 42.10 F ATOM 9190 C PHE F 43 83.397 76.000 66.520 1.00 42.10 F ATOM 9190 C PHE F 43 83.397 76.000 66.520 1.00 42.10 F ATOM 9190 C PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9190 C PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9190 C PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9190 C PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9190 C PHE F 43 83.897 76.500 66.525 1.00 39.84 F ATOM 9191 N CYS F 44 82.796 77.581 66.973 1.00 40.53 F ATOM 9192 CA CYS F 44 82.796 77.581 66.973 1.00 40.53 F ATOM 9193 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.55 F ATOM 9195 CB HJS F 45 83.667 82.172 66.305 1.00 39.84 F ATOM 9195 CB HJS F 45 83.667 82.172 66.305 1.00 39.76 F ATOM 9190 CC CYS F 45 83.667 82.172 66.305 1.00 40.88 F ATOM 9200 CG HJS F 45 83.667 82.172 66.305 1.00 39.76 F ATOM 9200 CG HJS F 45 83.667 82.172 66.305 1.00 39.94 F ATOM 9200 CG HJS F 45 83.668 82.192 66.505 1.00 39.94 F ATOM 9201 CD HJS F 45 83.668 82.192 63.000 30.000 39.94 F ATOM 9201 CG ANN F 46 83.000 83.000 66.000 1.000 39.94 F ATOM 9202 CD HJS F 47 88.896 82.000 63.899 1.00 44.11 F ATOM 9201 CD ANN F 46 83.900	-	9176	CG1	ILE	F	42	81.040	70.062	67.872	1.00 31.94	F
ATOM 9179 O ILE F 42 81.462 73.920 69.981 1.00 34.58 F ATOM 9180 N PHE F 43 83.276 74.133 68.625 1.00 40.15 F ATOM 9181 CA PHE F 43 83.276 74.133 68.625 1.00 37.57 F ATOM 9181 CA PHE F 43 84.757 75.846 69.528 1.00 37.57 F ATOM 9183 CG PHE F 43 84.757 73.841 70.900 1.00 37.57 F ATOM 9184 CD1 PHE F 43 85.320 73.841 70.900 1.00 39.96 F ATOM 9185 CD2 PHE F 43 84.850 75.158 70.836 1.00 39.96 F ATOM 9186 CE1 PHE F 43 85.320 73.841 70.900 1.00 40.49 F ATOM 9186 CE1 PHE F 43 85.320 73.841 70.900 1.00 40.49 F ATOM 9186 CZ PHE F 43 84.991 73.842 73.242 1.00 40.63 F ATOM 9188 CZ PHE F 43 84.991 73.848 73.200 1.00 35.43 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.96 F ATOM 9190 O PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9191 N CYS F 44 82.796 77.561 67.667 1.00 39.38 F ATOM 9191 N CYS F 44 82.796 77.561 67.667 1.00 39.38 F ATOM 9193 C C CYS F 44 83.115 79.913 66.973 1.00 41.58 F ATOM 9193 C C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9196 CG CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9197 N HTS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9197 N HTS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9199 CB HIS F 45 83.292 80.801 66.005 1.00 35.21 F ATOM 9190 CD HIS F 45 83.292 80.801 66.400 51.00 35.21 F ATOM 9190 CD HIS F 45 83.292 80.801 66.400 51.00 35.21 F ATOM 9201 CD2 HIS F 45 83.292 80.801 66.400 51.00 35.21 F ATOM 9202 ND1 HIS F 45 83.693 82.118 65.227 1.00 47.68 F ATOM 9201 CD2 HIS F 45 83.693 82.118 65.227 1.00 47.68 F ATOM 9201 CD2 HIS F 45 83.695 82.118 65.237 1.00 40.93 F ATOM 9201 CD2 HIS F 45 83.695 82.118 65.237 1.00 40.93 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 39.94 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 39.94 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 39.94 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 39.94 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 40.91 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 40.91 F ATOM 9202 ND1 HIS F 45 86.027 82.899 64.105 1.00 40.91 F ATOM 9202 ND1 HIS	MOTA	9177		_		42	79.741	69.572	67.315	1.00 32.41	F
ATOM 9180 N PHE F 43 83.276 74.133 68.625 1.00 40.15 F ATOM 9181 CA PHE F 43 83.439 75.571 68.823 1.00 39.76 F ATOM 9182 CB PHE F 43 84.880 75.158 70.836 1.00 37.57 F ATOM 9183 CG PHE F 43 84.880 75.158 70.836 1.00 37.57 F ATOM 9184 CD1 PHE F 43 84.880 73.158 70.836 1.00 38.48 F ATOM 9185 CD2 PHE F 43 84.880 73.841 70.900 1.00 39.96 F ATOM 9185 CD2 PHE F 43 84.891 75.803 72.013 1.00 41.38 F ATOM 9186 CE1 PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9187 CE2 PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9188 CZ PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9189 C PHE F 43 84.538 75.142 73.242 1.00 35.43 F ATOM 9189 C PHE F 43 84.538 75.142 73.242 1.00 39.77 F ATOM 9190 O PHE F 43 83.397 76.000 66.520 1.00 39.77 F ATOM 9191 N CVS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9192 CA CVS F 44 82.724 78.492 66.535 1.00 39.84 F ATOM 9193 C CVS F 44 83.271 80.200 68.653 1.00 40.53 F ATOM 9194 O CVS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CVS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9196 CB ATIS F 45 83.292 80.801 66.903 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.903 1.00 47.68 F ATOM 9198 CB HIS F 45 83.292 80.801 66.905 1.00 33.76 F ATOM 9199 CB HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9199 CB HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9199 CB HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9200 CG HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9201 CD2 HIS F 45 83.292 80.801 66.005 1.00 30.76 F ATOM 9202 ND1 ATOM 920 CG HIS F 45 83.295 82.118 65.237 1.00 30.98 F ATOM 920 CD HIS F	MOTA	9178	C	ILE	F	42	82.316	73.425	69.224	1.00 37.57	F
ATOM 9181 CA PHE F 43 84.757 75.571 68.823 1.00 37.57 F ATOM 9183 CG PHE F 43 84.757 75.846 69.528 1.00 37.57 F ATOM 9183 CG PHE F 43 84.880 75.158 70.836 1.00 38.96 F ATOM 9185 CD2 PHE F 43 84.880 75.158 70.836 1.00 39.96 F ATOM 9185 CD2 PHE F 43 84.891 75.803 72.013 1.00 41.38 F ATOM 9186 CE1 PHE F 43 85.320 73.841 70.900 1.00 40.49 F ATOM 9187 CE2 PHE F 43 84.891 75.803 72.013 1.00 41.38 F ATOM 9186 CE1 PHE F 43 84.891 75.803 72.013 1.00 40.49 F ATOM 9187 CE2 PHE F 43 84.897 73.818 73.300 1.00 35.43 F ATOM 9188 CZ PHE F 43 84.897 73.818 73.300 1.00 35.43 F ATOM 9189 C PHE F 43 83.394 76.000 66.520 1.00 42.10 F ATOM 9190 O PHE F 43 83.394 76.000 66.520 1.00 42.10 F ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9192 CA CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9193 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9193 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.315 78.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.315 78.913 66.973 1.00 47.68 F ATOM 9196 CB CYS F 44 83.315 78.913 66.973 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 35.21 F ATOM 9198 CA HIS F 45 83.667 82.172 66.505 1.00 35.21 F ATOM 9190 CB HIS F 45 83.667 82.172 66.505 1.00 35.21 F ATOM 9190 CB HIS F 45 83.667 82.172 66.505 1.00 35.21 F ATOM 9200 CG HIS F 45 85.963 82.118 65.207 1.00 40.88 F ATOM 9201 CD2 HIS F 45 86.758 81.016 66.005 1.00 35.21 F ATOM 9202 ND1 HIS F 45 86.758 81.016 66.005 1.00 37.14 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 37.14 F ATOM 9202 CD HIS F 45 86.758 81.016 65.016 1.00 37.14 F ATOM 9202 CD HIS F 45 86.758 81.016 65.016 1.00 37.14 F ATOM 9202 CD HIS F 45 86.758 81.016 65.016 1.00 37.14 F ATOM 9202 CD HIS F 45 86.758 81.016 65.016 1.00 37.14 F ATOM 9202 CD HIS F 45 86.758 81.016 65.016 1.00 37.14 F ATOM 9202 CD HIS F 45 86.758 81.006 64.027 71.00 39.88 F ATOM 9202 CD HIS F 46 81.929 80.801 66.005 1.00 37.43 F ATOM 9202 CD HIS F 46 81.929 80.801 66.005 1.00 37.43 F ATOM 9202 CD HIS F 46 81.929 80.801 66.005 1.00 37.44 F ATOM 9202 CD ASP F 47 85.5	MOTA	9179	0	ILE	F	42	81.462	73.920	69.981	1.00 34.58	F
ATOM 9182 CB PHE F 43 84.757 75.846 69.528 1.00 37.57 F ATOM 9183 CG PHE F 43 84.880 75.158 70.836 1.00 38.48 F ATOM 9184 CDL PHE F 43 85.320 73.841 70.900 1.00 39.96 F ATOM 9185 CD2 PHE F 43 84.891 73.803 1.00 40.49 F ATOM 9186 CE2 PHE F 43 84.531 73.164 72.123 1.00 40.49 F ATOM 9187 CE2 PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9188 CZ PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9189 C PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9190 O PHE F 43 83.897 76.000 66.520 1.00 39.77 F ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.88 F ATOM 9192 CA CYS F 44 83.151 79.913 66.973 1.00 40.53 F ATOM 9194 O CYS F 44 83.151 79.913 66.973 1.00 40.53 F ATOM 9195 CB CYS F 44 83.371 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 83.371 80.200 68.163 1.00 41.58 F ATOM 9196 SG CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9199 CB HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9190 CD HIS F 45 85.179 82.311 66.296 1.00 30.76 F ATOM 9201 CD2 HIS F 45 85.179 82.311 66.296 1.00 30.76 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.015 1.00 30.76 F ATOM 9205 C HIS F 45 86.958 81.016 65.015 1.00 30.76 F ATOM 9207 N ASN F 46 81.255 87.774 81.00 40.88 F ATOM 9207 N ASN F 46 81.255 87.774 81.00 40.89 F ATOM 9207 N ASN F 46 81.255 87.774 81.00 40.40 40.90 F ATOM 9207 C ASN F 46 81.255 87.775 81.00 44.1	MOTA	9180	N	PHE	F	43	83.276	74.133	68.625	1.00 40.15	F
ATOM 9183 CG PHE F 43 84.880 75.158 70.836 1.00 39.96 F ATOM 9184 CDI PHE F 43 85.320 73.841 70.900 1.00 39.96 F ATOM 9186 CEI PHE F 43 84.491 75.803 72.013 1.00 40.438 P ATOM 9186 CEI PHE 43 84.581 75.142 73.300 1.00 30.63 F ATOM 9189 C PHE F 43 84.979 73.818 73.300 1.00 99.77 F ATOM 9190 O PHE F 43 83.897 76.000 66.520 1.00 39.38 F ATOM 9190 O PHE F 43 83.897 76.000 66.520 1.00 39.38 F ATOM 9193 C CYS F <td>MOTA</td> <td>9181</td> <td>CA</td> <td>PHE</td> <td>F</td> <td>43</td> <td>83.439</td> <td>75.571</td> <td>68.823</td> <td>1.00 39.76</td> <td>F</td>	MOTA	9181	CA	PHE	F	43	83.439	75.571	68.823	1.00 39.76	F
ATOM 91.84 CD1 PHE F 43 85.320 73.841 70.900 1.00 39.96 F ATOM 91.85 CD2 PHE F 43 84.91 75.803 72.0123 1.00 41.38 F ATOM 91.87 CE2 PHE F 43 84.538 75.142 73.242 1.00 40.49 F ATOM 91.89 C PHE F 43 84.979 73.818 73.3042 1.00 40.63 F ATOM 91.90 O PHE F 43 83.997 76.000 66.520 1.00 39.38 F ATOM 91.91 N CYS F 44 82.726 77.581 67.667 1.00 39.38 F ATOM 91.91 C CYS F 44 83.211 80.200 66.535 1.00 39.38 F ATOM 91.92 CB CYS F 44 83.211 80.200 66.535 1.	ATOM	9182	CB	PHE	F	43	84.757		69.528	1.00 37.57	F
ATOM 9185 CD2 PHE F 43 84.491 75.803 72.013 1.00 41.38 F ATOM 9186 CE2 PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9188 CZ PHE F 43 84.979 73.818 73.300 1.00 35.43 F ATOM 9190 O PHE F 43 83.997 76.000 66.520 1.00 39.38 F ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9192 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9193 C CYS F 44 83.115 79.913 66.973 1.00 41.58 F ATOM 9195 CB CYS		9183	CG		F	43	84.880	75.158	70.836	1.00 38.48	F
ATOM 9186 CEL PHE F 43 85,373 73.164 72.123 1.00 40.49 F ATOM 9187 CE2 PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9189 C PHE F 43 84.979 73.818 73.300 1.00 39.77 F ATOM 9190 O PHE F 43 83.897 76.000 66.520 1.00 49.10 P ATOM 9191 N CYS F 44 82.796 77.581 66.535 1.00 39.38 F ATOM 9193 C CYS F 44 83.271 80.200 66.535 1.00 39.38 F ATOM 9194 C CYS F 44 83.211 80.200 66.1535 1.00 30.56 F ATOM 9196 CB CYS	ATOM		CD1	PHE	F	43	85.320	73.841	70.900	1.00 39.96	F
ATOM 9187 CE2 PHE F 43 84.538 75.142 73.242 1.00 40.63 F ATOM 9188 CZ PHE F 43 84.979 73.818 73.300 1.00 35.43 F ATOM 9190 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9190 N CYS F 44 82.724 78.492 66.535 1.00 39.84 F ATOM 9193 C CYS F 44 82.724 78.492 66.535 1.00 39.84 F ATOM 9195 CB CYS F 44 83.211 79.913 66.955 1.00 39.38 F ATOM 9195 CB CYS F 44 83.211 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00		9185			F	43	84.491	75.803	72.013	1.00 41.38	F
ATOM 9188 CZ PHE F 43 83.934 76.404 67.561 1.00 35.43 F ATOM 9199 C PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9190 N PHE F 43 83.897 76.000 66.520 1.00 39.37 P ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9192 CA CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9193 C CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9193 C CYS F 44 83.215 79.913 66.973 1.00 40.53 F ATOM 9194 O CYS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00 41.58 F ATOM 9196 SG CYS F 44 81.318 78.491 65.961 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 35.21 F ATOM 9199 CB HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9202 NDI HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9202 NDI HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9202 NDI HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9202 NDI HIS F 45 86.758 81.016 65.016 1.00 39.21 F ATOM 9202 CH HIS F 45 86.758 81.016 65.016 1.00 39.21 F ATOM 9202 CH HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9204 NE2 HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9205 C HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.94 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.98 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.98 F ATOM 9208 CA ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.937 88.595 64.805 1.00 39.94 F ATOM 9210 CG ASN F 46 81.937 88.595 64.805 1.00 39.94 F ATOM 9211 ODI ASN F 46 81.931 85.959 64.804 1.00 41.13 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.931 85.959 64.805 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.93		9186				43	85.373	73.164		1.00 40.49	F
ATOM 9189 C PHE F 43 83.394 76.404 67.561 1.00 39.77 F ATOM 9190 O PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9192 CA CYS F 44 82.794 77.581 67.667 1.00 39.38 F ATOM 9193 C CYS F 44 82.794 77.581 67.667 1.00 39.38 F ATOM 9194 O CYS F 44 83.15 79.913 66.535 1.00 39.84 F ATOM 9195 CB CYS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9196 SG CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9197 N HIS F 45 83.292 80.801 65.005 1.00 35.21 F ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9200 CG HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.758 81.016 65.016 1.00 30.76 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 39.21 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 39.21 F ATOM 9206 O HIS F 45 83.251 83.016 65.135 1.00 39.88 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9201 CD2 HIS F 45 83.251 83.016 65.135 1.00 37.14 F ATOM 9202 ND ASN F 46 83.070 84.304 65.401 1.00 39.98 F ATOM 9203 CE HIS F 45 83.251 83.016 65.135 1.00 37.14 F ATOM 9204 NE2 HIS F 45 83.251 83.016 65.135 1.00 37.14 F ATOM 9205 C ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9206 O HIS F 45 83.251 83.016 65.135 1.00 37.14 F ATOM 9210 CD2 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 CD ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.83 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.83 F ATOM 9212 CD ASN F 46 81.235 87.358 64.183 1.00 44.81 F ATOM 9212 CD ASN F 46 81.235 87.358 64.183 1.00 44.81 F ATOM 9212 CD ASN F 46 81.235 87.358 64.183 1.00 44.81 F ATOM 9212 CD ASN F 46 81.235 87.358 64.10 NO 41.51 F ATOM 9221 CD ASN F 46 81.235 87.35								75.142	73.242	1.00 40.63	F
ATOM 9191 O PHE F 43 83.897 76.000 66.520 1.00 42.10 F ATOM 9192 CA CYS F 44 82.796 77.581 67.667 1.00 39.84 F ATOM 9192 CA CYS F 44 82.724 78.492 66.535 1.00 39.84 F ATOM 9193 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9194 O CYS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9196 SG CYS F 44 80.664 76.852 65.512 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 37.74 F ATOM 9200 CG HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.598 81.016 65.237 1.00 37.14 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CEI HIS F 45 86.758 81.016 65.016 1.00 39.21 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 39.21 F ATOM 9206 C HIS F 45 83.251 83.016 65.135 1.00 39.94 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.68 F ATOM 9208 CA ASN F 46 83.070 84.304 65.401 1.00 39.98 F ATOM 9209 CB ASN F 46 81.971 86.445 65.125 1.00 37.14 F ATOM 9209 CB ASN F 46 81.971 86.445 65.125 1.00 37.14 F ATOM 9211 CD1 ASN F 46 81.971 86.445 65.125 1.00 37.98 F ATOM 9212 CD ASN F 46 81.971 86.445 65.125 1.00 37.99 F ATOM 9212 CD ASN F 46 81.971 86.445 65.125 1.00 39.98 F ATOM 9212 CD ASN F 46 81.971 86.445 65.125 1.00 39.98 F ATOM 9212 CD ASN F 46 81.971 86.445 65.125 1.00 45.58 F ATOM 9212 CD ASN F 46 81.971 86.445 65.125 1.00 45.58 F ATOM 9212 CD ASN F 46 81.971 86.445 66.183 1.00 45.58 F ATOM 9212 CD ASN F 46 81.971 86.445 66.183 1.00 45.58 F ATOM 9212 CD ASN F 46 81.971 86.445 66.191 1.00 39.99 F ATOM 9212 CD ASN F 46 81.971 86.445 66.191 1.00 49.10 F ATOM 9212 CD ASN F 47 85.613 85.794 66.183 1.00 47.40 F ATOM 9212 CD ASN F 47 85.513 86.477 61.974 1.00 49.87 F ATOM 9212 CD ASN F 47 85.513 86.477 61.974 1.00 49.87 F ATOM 9212 CD ASN F 47 85.513 86.677 1.00 47.40 F ATOM 9212 CD ASP F 47 85.513 86.677 1.00 47.40 F ATOM 9212 CD ASP F 47 85.566 80.05 60.05 61.901 1.00 49.10 F ATOM 9222 CD ASP F 47 85.566 90.035 59.38						43	84.979	73.818	73.300	1.00 35.43	F
ATOM 9191 N CYS F 44 82.796 77.581 67.667 1.00 39.38 F ATOM 9192 CA CYS F 44 82.724 78.492 66.535 1.00 39.38 F ATOM 9193 C CYS F 44 83.115 79.913 66.6973 1.00 40.53 F ATOM 9194 O CYS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00 47.68 F ATOM 9196 SG CYS F 44 81.318 78.491 65.961 1.00 47.68 F ATOM 9197 N HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9200 CG HIS F 45 86.027 82.311 66.496 1.00 30.76 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9202 ND1 HIS F 45 86.027 82.859 64.105 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.237 1.00 37.14 F ATOM 9206 O HIS F 45 83.251 83.016 65.135 1.00 37.14 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.91 F ATOM 9208 CA ASN F 46 81.971 86.436 64.09 1.00 39.94 F ATOM 9208 CA ASN F 46 81.971 86.436 65.401 1.00 39.98 F ATOM 9208 CA ASN F 46 81.971 86.435 65.126 1.00 39.98 F ATOM 9210 CG ASN F 46 81.971 86.435 66.401 1.00 39.38 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 37.14 F ATOM 9211 CD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9213 C ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9214 C ASN F 46 84.981 85.959 64.586 1.00 48.81 F ATOM 9215 N ASP F 47 85.613 85.867 60.582 1.00 45.39 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9218 CA ASP F 47 85.613 85.867 60.582 1.00 44.87 F ATOM 9210 CC ASP F 47 85.501 83.534 60.00 7 1.00 47.40 F ATOM 9212 CD ASP F 47 85.501 83.534 60.00 7 1.00 47.40 F ATOM 9221 CB ASP F 47 85.501 83.534 60.00 7 1.00 47.40 F ATOM 9222 CD ASP F 47 85.501 83.534 60.00 7 1.00 47.40 F ATOM 9222 CD ASP F 47 85.501 83.534 60.00 7 1.00 49.87 F ATOM 9222 CD ASP F 47 85.506 90.035 59.384 1.00 49.10 F ATOM 9222 CD ASP F 48 84.355 8										1.00 39.77	
ATOM 9193 C CYS F 44 82.724 78.492 66.535 1.00 39.84 F ATOM 9194 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9194 C CYS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 80.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 80.664 76.852 65.512 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9198 CA HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9201 CD2 HIS F 45 85.179 82.311 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.578 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9204 ME2 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9205 C HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9205 C HIS F 45 86.274 81.083 63.801 1.00 39.21 F ATOM 9205 C HIS F 45 83.251 83.016 65.161 1.00 39.21 F ATOM 9205 C HIS F 45 83.251 83.016 65.165 1.100 36.46 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.98 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.99 F ATOM 9209 CB ASN F 46 81.971 86.445 65.125 1.00 44.11 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 44.11 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 47.43 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 47.43 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 47.43 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 47.43 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 47.43 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 47.40 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 44.11 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 44.11 F ATOM 9210 CG ASN F 46 81.971 86.445 66.1916 1.00 44.11 F ATOM 9210 CG ASN F 46 81.971 86.445 66.1916 1.00 44.11 F ATOM 9210 CD ASN F 46 81.971 86.445 66.1916 1.00 44.11 F ATOM 9210 CD ASN F 46 81.971 86.495 60.644 1.00 44.27 F ATOM 9210 CD ASN F 47 85.613 85.996 60.00 60.00 51.31 F ATOM 9210 CD ASP F 47 85.613 85.8									66.520	1.00 42.10	F
ATOM 9194 C CYS F 44 83.115 79.913 66.973 1.00 40.53 F ATOM 9194 O CYS F 44 83.271 80.200 68.163 1.00 41.58 F ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9196 SG CYS F 44 80.664 76.852 65.512 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.61 66.005 1.00 38.76 F ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.677 82.112 66.496 1.00 30.76 F ATOM 9200 CG HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.027 82.859 64.105 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.846 82.192 63.261 1.00 37.14 F ATOM 9203 CE1 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9207 N ASN F 46 83.095 82.506 64.027 1.00 39.88 F ATOM 9208 CA ASN F 46 83.095 82.506 64.027 1.00 39.94 F ATOM 9209 CB ASN F 46 83.095 82.506 64.027 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 CD1 ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9211 CD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9212 ND ASN F 46 84.025 85.866 60.007 1.00 49.55 F ATOM 9222 C ASN F 47 85.364 86.477 61.974 1.00 48.14 F ATOM 9221 C ASN F 47 85.364 86.975 88.667 60.582 1.00 49.87 F ATOM 9222 C ASP										1.00 39.38	F.
ATOM 9194 O CYS F 44 81.318 78.491 65.961 1.00 41.58 F ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9196 SG CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9201 CD2 HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 38.71 F ATOM 9201 NHIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9204 NE2 HIS F 45 86.758 81.016 65.016 1.00 39.21 F ATOM 9204 NE2 HIS F 45 86.864 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 39.21 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 39.21 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9211 ODL ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9211 ODL ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 ODL ASN F 46 81.235 87.358 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 81.274 87.726 63.125 1.00 37.43 F ATOM 9213 C ASN F 46 81.274 87.726 63.125 1.00 45.58 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 44.11 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 48.14 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 48.14 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 48.14 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 48.14 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 48.14 F ATOM 9217 CB ASP F 47 85.496 88.006 61.916 1.00 44.27 F ATOM 9220 CD ASP F 47 85.496 88.006 61.916 1.00 44.27 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 44.27 F ATOM 9222 C ASP F 47 85.496 88.006 61.916 1.00 44.27 F ATOM 9222 C ASP F 47 85.496 88.006 61.90											
ATOM 9195 CB CYS F 44 81.318 78.491 65.961 1.00 43.15 F ATOM 9196 SG CYS F 44 80.664 76.852 65.512 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9199 CB HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9200 CG HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9209 CB ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 82.689 85.303 64.409 1.00 39.98 F ATOM 9201 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9213 C ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 44.83 F ATOM 9213 C ASN F 46 84.023 85.794 64.383 91.00 44.83 F ATOM 9212 CG ASN F 46 84.023 85.794 64.383 91.00 44.13 F ATOM 9212 CC ASN F 46 84.023 85.794 64.383 91.00 44.83 F ATOM 9212 C ASN F 46 84.023 85.794 64.383 91.00 44.83 F ATOM 9212 CC ASN F 46 84.023 85.794 64.383 91.00 44.13 F ATOM 9212 CC ASN F 46 84.023 85.794 60.383 91.00 44.83 F ATOM 9212 CC ASN F 46 84.023 85.794 60.383 91.00 44.13 F ATOM 9212 CC ASN F 46 84.023 85.794 60.383 91.00 44.83 F ATOM 9212 CC ASN F 46 84.023 85.794 60.383 91.00 44.83 F ATOM 9212 CC ASN F 46 84.023 85.794 60.383 91.00 44.83 F ATOM 9212 CC ASN F 46 84.023 85.794 60.383 91.00 44.83 F ATOM 9222 CC ASN F 47 85.501 83.534 60.007 1.00 44.83 F ATOM 9222 CC ASN F 47 85.501 83.534 60.007 1.00 44.83 F ATOM 9222 CC ASN F											
ATOM 9196 SG CYS F 44 80.664 76.852 65.512 1.00 47.68 F ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 30.76 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9201 CD2 HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9202 ND1 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.095 82.506 64.027 1.00 39.21 F ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.99 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 CD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.027 87.742 63.825 1.00 45.58 F ATOM 9213 C ASN F 46 81.027 87.742 64.567 1.00 37.43 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 44.11 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 44.11 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 44.11 F ATOM 9215 C ASN F 46 84.023 85.794 63.839 1.00 44.83 F ATOM 9216 CA ASN F 46 84.981 85.959 64.566 1.00 37.43 F ATOM 9216 CA ASN F 46 84.981 85.959 64.566 1.00 37.43 F ATOM 9216 CA ASN F 46 84.981 85.959 64.566 1.00 48.89 F ATOM 9216 CA ASN F 47 85.613 85.867 60.562 1.00 46.39 F ATOM 9219 OD1 ASN F 46 84.981 85.959 64.566 1.00 49.87 F ATOM 9212 C ASN F 47 85.513 85.867 60.562 1.00 47.40 F ATOM 9212 C ASN F 47 85.513 85.8662 1.00 64.4 1.00 49.87 F ATOM 9221 C ASN F 47 85.513 85.867 60.564 1.00 49.87 F ATOM 9222 C ASP F 47 85.546 80.06 61.916 1.00 52.11 F ATOM 9222 C C ASP F 47 85.595 88.565 61.931 1.00 52.11 F ATOM 9222 C C ASP F 47 85.595 88.565 61.931 1.00 64.65 F ATOM 9222 C C TYR F 48 84.366 90.334 59.55 59.38 1.00 67.04 F ATOM 9222 C C TYR F 48 84.366 90.334 59.55 59.38 1.00 64.64 F ATOM 9222											
ATOM 9197 N HIS F 45 83.292 80.801 66.005 1.00 38.76 F ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9200 CG HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9201 CD2 HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.051 82.51 83.016 65.135 1.00 36.46 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.971 86.445 65.125 1.00 43.78 F ATOM 9211 OD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.27 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9212 C ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9212 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 49.17 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C ASP F 47 85.606 90.035 59.384 1.00 67.04 F ATOM 9222 C CB TYR F 48 84.315 88.682 61.860 1.00 55.53 F ATOM 9222 C CB TYR F 48 84.316 90.035 59.384 1.00 67.04 F ATOM 9222 C CB TYR F 48 84											
ATOM 9198 CA HIS F 45 83.667 82.172 66.305 1.00 35.21 F ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9200 CG HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9202 ND1 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 C HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.94 F ATOM 9208 CA ASN F 46 81.971 86.445 65.126 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9211 OD1 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.981 85.994 64.567 1.00 45.58 F ATOM 9213 C ASN F 46 84.981 85.995 64.586 1.00 45.58 F ATOM 9214 O ASN F 46 84.981 85.995 64.586 1.00 44.83 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9215 N ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9212 C ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9212 C ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9212 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C C ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 C C ASP F 47 85.506 90.035 59.384 1.00 67.04 F ATOM 9222 C C ASP F 47 85.606 90.035 59.384 1.00 67.04 F ATOM 9225 CB TYR F 48 84.346 9											
ATOM 9199 CB HIS F 45 85.179 82.311 66.496 1.00 30.76 F ATOM 9201 CD2 HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9202 ND1 HIS F 45 86.027 82.859 64.105 1.00 37.14 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 37.43 F ATOM 9212 ND2 ASN F 46 81.747 87.726 63.125 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9215 N ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 44.83 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9219 OD1 ASP F 47 85.613 85.867 60.582 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.613 85.867 60.582 1.00 47.40 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9222 C ASP F 47 85.613 85.867 60.582 1.00 49.87 F ATOM 9222 C ASP F 47 85.606 90.035 59.384 1.00 64.22 F ATOM 9222 C C ASP F 47 85.606 90.035 59.384 1.00 64.22 F ATOM 9222 C C ASP F 47 85.606 90.035 59.384 1.00 64.22 F ATOM 9222 C C TYR F 48 84.346 90.134 61.821 1.00 64.22 F ATOM 9222 C C TYR F 48 84.346 90.135 59.667 1.00 67.04 F ATOM 9222 C C TYR F 48 84.335 88.873 58.672 1.00 67.04 F ATOM 9222 C C TYR F 48 85.606 90.035 59.384 1.00 64.62 F ATOM 9222 C C TYR F 48 86											
ATOM 9200 CG HIS F 45 85.963 82.118 65.237 1.00 37.14 F ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 87.274 81.083 63.801 1.00 39.21 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.051 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 CD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.247 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 84.023 85.794 63.839 1.00 45.58 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 C ASN F 46 84.023 85.794 63.839 1.00 44.83 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 48.34 F ATOM 9216 CA ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9217 CB ASP F 47 85.384 86.477 61.974 1.00 44.83 F ATOM 9217 CB ASP F 47 85.184 86.477 61.974 1.00 44.83 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 47.40 F ATOM 9210 CD ASP F 47 85.613 85.867 60.582 1.00 47.40 F ATOM 9221 CD ASP F 47 85.511 84.423 60.644 1.00 44.27 F ATOM 9210 CD ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 CD ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 CD ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 CD ASP F 47 85.501 83.534 60.007 1.00 49.10 F ATOM 9222 CD ASP F 47 85.505 88.662 61.860 1.00 49.87 F ATOM 9222 CD ASP F 47 85.505 88.662 61.860 1.00 55.53 F ATOM 9222 CD ASP F 47 85.506 90.035 59.384 1.00 64.22 F ATOM 9222 CD ASP F 47 85.506 90.035 59.384 1.00 64.22 F ATOM 9222 CD ASP F 47 85.606 90.035 59.384 1.00 64.22 F ATOM 9222 CD ASP F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9222 CD TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9222 CD TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9222 CD TYR F 48 84.346 90.035 59.384 1.00 64.64 F ATOM 9222 CD TYR F 48 85.632											
ATOM 9201 CD2 HIS F 45 86.027 82.859 64.105 1.00 40.88 F ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.98 F ATOM 9208 CA ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.747 87.726 63.125 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 81.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.981 85.959 64.586 1.00 43.78 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 44.83 F ATOM 9215 N ASP F 47 84.911 86.020 62.534 1.00 44.83 F ATOM 9215 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9212 CD ASP F 47 85.501 83.534 60.007 1.00 49.87 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 49.87 F ATOM 9222 OD2 ASP F 47 86.511 84.423 60.644 1.00 44.27 F ATOM 9221 C ASP F 47 86.511 84.423 60.644 1.00 44.27 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C C ASP F 47 86.595 88.565 61.931 1.00 55.31 F ATOM 9222 C C ASP F 47 86.595 88.565 61.931 1.00 64.62 F ATOM 9222 C C TYR F 48 84.346 90.134 61.821 1.00 55.31 F ATOM 9222 C C TYR F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9222 C C TYR F 48 84.366 90.035 59.384 1.00 64.64 F ATOM 9222 C C TYR F 48 85.632 88.296 57.773 1.00 66.28 F				•							
ATOM 9202 ND1 HIS F 45 86.758 81.016 65.016 1.00 38.71 F ATOM 9203 CE1 HIS F 45 87.274 81.083 63.801 1.00 39.21 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.251 83.016 65.135 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 84.023 85.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.759 64.586 1.00 41.13 F ATOM 9213 C ASN F 46 84.023 85.959 64.586 1.00 41.13 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9210 CD ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9221 C ASP F 47 85.613 85.867 60.582 1.00 47.40 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 C ASP F 47 85.496 88.066 61.916 1.00 49.87 F ATOM 9222 C ASP F 47 85.496 88.682 61.860 1.00 52.11 F ATOM 9222 C ASP F 47 85.496 88.682 61.860 1.00 52.11 F ATOM 9222 C ASP F 47 85.496 88.682 61.861 1.00 52.11 F ATOM 9222 C ASP F 47 85.496 88.682 61.861 1.00 55.53 F ATOM 9222 C ASP F 47 85.595 88.565 61.931 1.00 49.10 F ATOM 9222 C ASP F 47 85.496 88.006 61.916 1.00 52.11 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 64.22 F ATOM 9225 CB TYR F 48 84.400 90.035 59.384 1.00 64.22 F ATOM 9226 CG TYR F 48 84.400 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.400 90.035 59.384 1.00 64.22 F ATOM 9228 CE1 TYR F 48 84.400 90.035 59.384 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.0035 59.384 1.00 66.66 F ATOM 9229 CD2 TYR F 48 86.323 90.0035 59.366 1.00 68.28 F											
ATOM 9203 CE1 HIS F 45 87.274 81.083 63.801 1.00 39.21 F ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9211 OD1 ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9212 ND2 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.83 F ATOM 9219 OD1 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9220 CD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.87 F ATOM 9222 C ASP F 47 85.501 83.534 60.007 1.00 49.87 F ATOM 9222 C C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C C C TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9225 CB TYR F 48 84.360 90.035 59.384 1.00 64.22 F ATOM 9226 CG TYR F 48 84.360 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.360 90.035 59.384 1.00 67.04 F ATOM 9228 CE1 TYR F 48 84.363 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 89.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 89.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F											
ATOM 9204 NE2 HIS F 45 86.846 82.192 63.226 1.00 37.14 F ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9219 OD1 ASP F 47 85.496 88.006 61.916 1.00 44.27 F ATOM 9220 OD2 ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9222 C ASP F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9224 CA TYR F 48 84.356 88.682 61.860 1.00 55.53 F ATOM 9225 CB TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9227 CD1 TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.336 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 86.32											
ATOM 9205 C HIS F 45 83.251 83.016 65.135 1.00 36.46 F ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CD ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9215 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9222 O ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9222 O ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9224 CA TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9225 CB TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9226 CG TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9227 CD1 TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9227 CD2 TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9227 CD2 TYR F 48 84.365 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CD2 TYR F 48 86.											
ATOM 9206 O HIS F 45 83.095 82.506 64.027 1.00 39.68 F ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 44.83 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9219 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9222 O ASP F 47 85.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9222 C ASP F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9224 CA TYR F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9225 CB TYR F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9225 CB TYR F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9226 CG TYR F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9227 CD1 TYR F 48 84.335 88.682 61.860 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 66.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9207 N ASN F 46 83.070 84.304 65.401 1.00 39.38 F ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9215 N ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9219 OD1 ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9219 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.911 1.00 49.87 F ATOM 9222 O ASP F 47 85.496 88.006 61.911 1.00 49.87 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9223 N TYR F 48 84.355 88.682 61.861 1.00 52.11 F ATOM 9224 CA TYR F 48 84.355 88.682 61.861 1.00 55.53 F ATOM 9225 CB TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9227 CD1 TYR F 48 84.355 88.682 61.860 1.00 55.53 F ATOM 9227 CD1 TYR F 48 84.335 88.873 58.672 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 64.22 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9208 CA ASN F 46 82.689 85.303 64.409 1.00 39.94 F ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9215 CA ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.300 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.300 90.627 60.396 1.00 55.53 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.66 F ATOM 9220 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9209 CB ASN F 46 81.971 86.445 65.126 1.00 43.78 F ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 64.586 1.00 38.92 F ATOM 9215 N ASP F 46 84.981 85.795 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 47.40 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 49.87 F ATOM 9222 O ASP F 47 85.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9224 CA TYR F 48 84.355 88.682 61.860 1.00 52.11 F ATOM 9225 CB TYR F 48 84.366 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.366 90.134 61.821 1.00 52.11 F ATOM 9226 CG TYR F 48 84.366 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.373 88.8296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9210 CG ASN F 46 81.235 87.358 64.183 1.00 44.11 F ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.366 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.100 90.627 60.396 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.100 90.627 60.396 1.00 64.22 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F											
ATOM 9211 OD1 ASN F 46 81.747 87.726 63.125 1.00 45.58 F ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 85.613 85.867 60.582 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.87 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9226 CG TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 64.64 F ATOM 9229 CD2 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9212 ND2 ASN F 46 80.027 87.742 64.567 1.00 37.43 F ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.346 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9213 C ASN F 46 84.023 85.794 63.839 1.00 41.13 F ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F											
ATOM 9214 O ASN F 46 84.981 85.959 64.586 1.00 38.92 F ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F											
ATOM 9215 N ASP F 47 84.111 86.020 62.534 1.00 44.83 F ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 68.28 F											
ATOM 9216 CA ASP F 47 85.384 86.477 61.974 1.00 48.14 F ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F											
ATOM 9217 CB ASP F 47 85.613 85.867 60.582 1.00 46.39 F ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.737 88.873 58.672 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F											
ATOM 9218 CG ASP F 47 86.111 84.423 60.644 1.00 44.27 F ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 84.737 88.873 58.672 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	MOTA	9217	CB	ASP	F						
ATOM 9219 OD1 ASP F 47 87.125 84.179 61.330 1.00 47.40 F ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28	MOTA	9218	CG	ASP	F	47	86.111			_	
ATOM 9220 OD2 ASP F 47 85.501 83.534 60.007 1.00 41.51 F ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	MOTA	9219	OD1	ASP	F	47 .					
ATOM 9221 C ASP F 47 85.496 88.006 61.916 1.00 49.87 F ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28	MOTA	9220	OD2	ASP	F	47				1.00 41.51	
ATOM 9222 O ASP F 47 86.595 88.565 61.931 1.00 49.10 F ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	MOTA		С	ASP	F	47					
ATOM 9223 N TYR F 48 84.355 88.682 61.860 1.00 51.31 F ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	MOTA	9222	0	ASP	F	47	86.595	88.565	61.931	1.00 49.10	
ATOM 9224 CA TYR F 48 84.346 90.134 61.821 1.00 52.11 F ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	MOTA	9223	N	TYR	F	48	84.355	88.682	61.860	1.00 51.31	
ATOM 9225 CB TYR F 48 84.100 90.627 60.396 1.00 55.53 F ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	MOTA	9224	CA	TYR	F	48	84.346	90.134	61.821	1.00 52.11	F
ATOM 9226 CG TYR F 48 85.066 90.035 59.384 1.00 64.22 F ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F						48	84.100	90.627	60.396	1.00 55.53	
ATOM 9227 CD1 TYR F 48 84.737 88.873 58.672 1.00 67.04 F ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F	ATOM					48	85.066	90.035	59.384	1.00 64.22	
ATOM 9228 CE1 TYR F 48 85.632 88.296 57.773 1.00 68.66 F ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F						48		88.873	58.672	1.00 67.04	
ATOM 9229 CD2 TYR F 48 86.323 90.608 59.166 1.00 64.64 F ATOM 9230 CE2 TYR F 48 87.230 90.034 58.269 1.00 68.28 F						48			57.773	1.00 68.66	F
						48				1.00 64.64	
ATOM 9231 CZ TYR F 48 86.874 88.876 57.581 1.00 68.66 F										1.00 68.28	F
	MOTA	9231	CZ	TYR	F	48	86.874	88.876	57.581	1.00 68.66	F

ATOM	9232	OH	TYR		48	87.760	88.267	56.728	1.00 68.74	F
MOTA	9233	С	TYR	F	48	83.262	90.633	62.762	1.00 51.91	F
ATOM	9234	0	TYR	F	48	82.256	91.214	62.328	1.00 54.25	F
ATOM	9235	. N	PRO	F	49	83.463	90.414	64.074	1.00 48.98	F
ATOM	9236	CD	PRO	F	49	84.675	89.810	64.653	1.00 50.70	. F
ATOM	9237	CA	PRO		49	82.535	90.813	65.133	1.00 50.04	F
ATOM	9238	CB	PRO	F	49	83.290	90.453	66.413	1.00 48.62	F
ATOM	9239	CG	PRO	F	49	84.717	90.435	66.007	1.00 48.81	F
MOTA	9240	C	PRO	F	49	82.080	92.269	65.102	1.00 53.96	F
MOTA	9241	0	PRO	F	49	80.881	92.537	65.007	1.00 54.22	F
ATOM	9242	N	GLU		50	83.036	93.199	65.159	1.00 55.66	F
MOTA	9243	CA	GLU	F	50	82.749	94.643	65.158	1.00 53.61	F
ATOM	9244	CB	GLU		50	84.038	95.454	65.023	1.00 46.52	F
MOTA	9245	CG	GLU		50	85.145	95.079	65.977	1.00 55.75	F
MOTA	9246	CD	GLU		50	85.831	93.777	65.600	1.00 63.20	F
MOTA	9247		GLU		50	85.654	93.309	64.447	1.00 64.70	F
ATOM	9248		GLU		50	86.564	93.226	66.454	1.00 64.13	F
ATOM	9249	C	GLU		50	81.765	95.179	64.109	1.00 52.68	F
ATOM	9250	0	GLÜ		50	81.199	96.250	64.297	1.00 55.19	F
ATOM	9251	N	THR		51	81.549	94.464	63.013	1.00 49.84	F
ATOM	9252	CA	THR		51	80.646	94.977	61.988	1.00 53.47	F
ATOM	9253	CB	THR		51	81.454	95.486	60.761	1.00 53.02	F
ATOM	9254		THR		51	81.741	94.406	59.858	1.00 49.48	F
ATOM	9255	CG2			51	82.774	96.054	61.234	1.00 54.99	F
ATOM	9256	C	THR		51	79.631	93.934	61.532	1.00 57.58	F
ATOM	9257	ō	THR		51	78.664	94.247	60.823	1.00 57.30	F
ATOM	9258	N	ILE		52	79.850	92.686	61.935	1.00 55.85	F
MOTA	9259	CA	ILE		52	78.934	91.636	61.545	1.00 50.11	F
ATOM	9260	CB	ILE		52	79.563	90.725	60.494	1.00 50.95	F
ATOM	9261	CG2	ILE		52	78.594	89.599	60.131	1.00 50.05	F
ATOM	9262	CG1			52	79.911	91.547	59.250	1.00 49.40	F
ATOM	9263		ILE		52	80.579	90.746	58.162	1.00 47.71	F
ATOM	9264	C	ILE		52	78.510	90.803	62.725	1.00 47.97	F
ATOM	9265	ō	ILE		52	79.320	90.465	63.578	1.00 46.12	F
ATOM	9266	N	THR		53	77.219	90.502	62.787	1.00 47.89	F
ATOM	9267	CA	THR		53	76.688	89.672	63.855	1.00 50.10	F
ATOM	9268	CB	THR		53	75.505	90.354	64.578	1.00 52.79	F
ATOM	9269		THR		53	76.011	91.280	65.552	1.00 48.04	F
ATOM	9270	CG2	THR	F	53	74.629	89.314	65.276	1.00 49.03	F
ATOM	9271	C	THR		53	76.236	88.352	63.249	1.00 49.60	F
MOTA	9272	0	THR	F	53	75.434	88.329	62.306	1.00 49.63	F
ATOM	9273	N	ASP	F	54	76.765	87.257	63.791	1.00 49.87	F
MOTA	9274	CA	ASP	F	54	76.441	85.918	63.301	1.00 50.24	F
ATOM	9275	CB	ASP		54	77.706	85.035	63.298	1.00 48.39	· F
MOTA	9276	CG	ASP		54	78.693	85.416	62.192	1.00 45.32	F
ATOM	9277	OD1			54	78.243	85.670	61.055	1.00 45.90	F
MOTA	9278		ASP		54	79.918	85.447	62.452	1.00 44.36	F
MOTA	9279	C	ASP		54	75.327	85.223	64.094	1.00 48.69	F
ATOM	9280	0	ASP		54	75.265	85.320	65.324	1.00 45.65	F
MOTA	9281	N	TYR		55	74.461	84.519	63.363	1.00 50.52	F
ATOM	9282	CA	TYR		55	73.331	83.767	63.928	1.00 50.37	F
ATOM	9283	CB	TYR		55	72.029	84.208	63.274	1.00 50.69	F
ATOM	9284	CG	TYR		55	71.762	85.687	63.366	1.00 54.96	F
MOTA	9285		TYR		55	71.346	86.399	62.236	1.00 53.99	F
ATOM	9286		TYR		55	71.107	87.761	62.291	1.00 57.00	F
ATOM	9287		TYR		55	71.929	86.381	64.571	1.00 52.15	F
ATOM	9288	CE2			55	71.687	87.754	64.643	1.00 59.82	· F
ATOM	9289	CZ	TYR		55	71.278	88.440	63.491	1.00 59.09	F
				-						-

ATOM	9290	OH	TYR	F	55	71.054	89.800	63.521	1.00	53.63	F
ATOM	9291	C	TYR	F	55	73.486	82.263	63.704	1.00	46.89	F
MOTA	9292	0	TYR	F	55	73.431	81.790	62.570	1.00	45.92	F
MOTA	9293	N	VAL	F	56	73.670	81.522	64.790	1.00	45.33	F
MOTA	9294	CA	VAL	F	56	73.828	80.078	64.714		44.46	F
MOTA	9295	CB	VAL	F	56	74.998	79.626	65.564		46.20	F
ATOM	9296		VAL		56	75.108	78.108	65.530		45.80	F
ATOM	9297	CG2	VAL		56	76.260	80.261	65.033		47.31	F
MOTA	9298	С	VAL		56	72.565	79.360	65.164		43.21	F
MOTA	9299	0	VAL		56	72.001	79.653	66.206	•	45.21	F
ATOM	9300	N	THR		57	72.154	78.376	64.387		43.55	F
MOTA	93'01	CA	THR		57	70.917	77.659	64.656		40.66	F
ATOM	9302	CB	THR		57	69.886	78.152	63.631		33.53	F
ATOM	9303	OG1	THR		57	68.588	78.182	64.199		34.79	F
ATOM	9304	CG2	THR		57	69.886	77.263	62.437		21.98	F
ATOM	9305	C	THR		57	71.091	76.133	64.508		40.60	F
ATOM	9306	Ō	THR	_	57	71.965	75.688	63.767		42.05	F
MOTA	9307	N	LEU		58	70.283	75.337	65.215		38.61	F
ATOM	9308	CA	LEU		58	70.357	73.882	65.054		41.47	F
ATOM	9309	CB	LEU		58	70.056	73.131	66.357		39.80	F
ATOM	9310	CG	LEU		58	69.934	71.602	66.154		38.42	F
ATOM	9311		LEU	•	58	71.288	71.027	65.764		34.72	F
ATOM	9312		LEU		58 -	69.430	70.919	67.411		32.56	F
ATOM	9313	C	LEU		58	69.324	73.485	63.990		42.93	F
ATOM	9314	ŏ	LEU		58	68.216	73.041	64.311		44.09	F
ATOM	9315	N	GLN		59	69.715	73.657	62.727		41.95	F
ATOM	9316	CA	GLN		59	68.889	73.369	61.556		41.80	F
ATOM	9317	CB	GLN		59	69.776	73.398	60.308		48.74	F
ATOM	9318	CG	GLN		59	69.257	74.221	59.128		59.59	F
ATOM	9319	CD	GLN		59	67.850	73.851	58.708		66.26	F
ATOM	9320	OE1	GLN		59	66.869	74.294	59.310		70.05	F
ATOM	9321	NE2	GLN	-	59		73.026	57.673		71.52	F
ATOM	9322	C	GLN		59	68.147	72.028	61.605		39.89	F
MOTA	9323	ō	GLN		59	66.941	71.965	61.356		37.86	F
MOTA	9324	N	ARG		60	68.881	70.960	61.911		37.41	F
MOTA	9325	CA	ARG		60	68.315	69.616	61.974		35.64	F
ATOM	9326	CB	ARG		60	68.231		60.559		35.40	F
ATOM	9327	CG	ARG		60	67.434	67.758	60.407		43.14	F
ATOM	9328	CD	ARG	F	60	67.551	67.196	58.987		53.81	F
MOTA	9329	NE	ARG	F	60	67.924	68.223		1.00	71.63	F
MOTA	9330	CZ	ARG		60	67.167	69.269	57.663	1.00	78.01	F
MOTA	9331	NH1	ARG	F	60	65.967	69.450	58.212	1.00	80.35	F
MOTA	9332	NH2	ARG	F	60	67.616	70.153	56.775	1.00	77.33	F
MOTA	9333	C	ARG		60	69.175	68.710	62.860		36.20	F
MOTA	9334	0	ARG	F	60	70.372	68.934	63.030		42.72	F
MOTA	9335	N	GLY	F	61	68.551	67.695	63.437		3359	F
MOTA	9336	CA	GLY		61	69.252	66.761	64.296	1.00	32.24	F
MOTA	9337	C	GLY		61	68.698	65.399	63.944		36.29	F
MOTA	9338	0	GLY '		61	67.488	65.202	63.980		38.35	F
MOTA	9339	N	SER		62	69.571	64.457	63.604	1.00	35.65	F
MOTA	9340	CA	SER		62	69.119	63.141	63.208	1.00	33.23	F
MOTA	9341	CB	SER		62	69.277	62.987	61.704		35.05	F
MOTA	9342	OG	SER		62	68.519	63.977	61.037		38.93	F
MOTA	9343	C	SER		62	69.852	62.030	63.904		37.88	F
MOTA	9344	0	SER		62	71.057	62.132	64.153		42.83	F
ATOM	9345	N	ALA		63	69.118	60.951	64.185		37.19	F
MOTA	9346	CA	ALA		63	69.657	59.780	64.876		31.80	F
MOTA	9347	CB	ALA		63	68.672	59.299	65.904		33.96	F
											_

MOTA	9348	C	ALA		63 .	69.979	58.650	63.921	1.00 28.53	F
MOTA	9349	0	ALA	F	63	69.353	58.520	62.885	1.00 28.53	F
ATOM	9350	N	TYR	F	64	70.961	57.834	64.293	1.00 27.17	F
ATOM	9351	CA	TYR	F	64	71.400	56.696	63.498	1.00 26.93	F
ATOM	9352	CB	TYR	F	64	72.629	57.072	62.654	1.00 29.13	F
ATOM	9353	CG	TYR	F	64	72.325	58.102	61.600	1.00 36.07	F
MOTA	93 54	CD1	TYR	F	64	72.348	59.469	61.899	1.00 38.07	F
MOTA	9355	CEl	TYR	F	64	71.950	60.416	60.963	1.00 38.21	F
ATOM	9356	CD2	TYR	F	64	71.908	57.715	60.333	1.00 34.82	F
ATOM	9357	CE2	TYR	F	64	71.509	58.650	59.397	1.00 36.11	F
MOTA	9358	CZ	TYR	F	64	71.527	59.993	59.714	1.00 42.45	F
MOTA	9359	OH	TYR		64	71.095	60.910	58.785	1.00 51.02	F
MOTA	9360	C	TYR		64	71.740	55.480	64.358	1.00 26.37	F
MOTA	9361	0	TYR		64	72.020	55.598	65.554	1.00 25.90	F
MOTA	9362	N	GLY		65	71.728	54.312	63.725	1.00 25.24	F
ATOM	9363	CA	GLY		65	72.031	53.075	64.415	1.00 24.65	F
MOTA	9364	C	GLY		65	71.254	52.917 .		1.00 29.04	F
MOTA	9365	0	GLY		65	70.037	53.198	65.784	1.00 28.86	· F
ATOM	9366	N	GLY		66	71.975	52.483	66.735	1.00 26.65	F
MOTA	9367	CA	GLY		66	71.363	52.258	68.025	1.00 29.12	F
MOTA	9368	C	GLY		66	70.588	53.435	68.546	1.00 30.54	F
MOTA	9369	0	GLY		66	69.475	53.283	69.012	1.00 34.98	F
ATOM	9370	N	VAL		67	71.164	54.621	68.466	1.00 31.58	F
ATOM	9371	CA	VAL		67	70.471	55.787	68.961	1.00 33.63	F
MOTA	9372	CB	VAL		67	71.183	57.064	68.543	1.00 34.48	F
ATOM ATOM	9373 9374	CG1	VAL VAL		67 67	70.259	58.257	68.766	1.00 32.71	F
ATOM	9374	CGZ	VAL			72.483	57.225	69.349	1.00 29.37	F
ATOM	9376	0	VAL		67 67	69.050	55.848	68.448	1.00 36.24	F
MOTA	9377	И	LEU		68	68.128 68.889	56.210 55.466	69.173 67.194	1.00 40.82	F
ATOM	9378	CA	LEU		68	67.607	55.499	66.510	1.00 37.51	F
ATOM	9379	CB	LEU		68	67.880	55.383	65.017	1.00 39.03	F
ATOM	9380	CG	LEU		68	66.793	55.646	63.988	1.00 37.37 1.00 31.34	F F
ATOM	9381	CD1			68	66.205	57.029	64.179	1.00 31.34	F
ATOM	9382		LEU		68	67.427	55.503	62.610	1.00 24.86	F
ATOM	9383	C	LEU		68	66.622	54.413	66.933	1.00 24.00	F
ATOM	9384	ō	LEU		68	65.411	54.632	66.994	1.00 41.09	F
ATOM	9385	N	SER		69	67.141	53.240	67.241	1.00 41.05	F
ATOM	9386	CA	SER		69	66.273	52.137	67.593	1.00 40.78	F
ATOM	9387	CB	SER		69	66.769	50.867	66.911	1.00 39.72	F
ATOM	9388	OG	SER	F	69	68.104	50.585	67.296	1.00 34.71	F
MOTA	9389	C	SER	F	69	66.108	51.854	69.069	1.00 40.56	. F
MOTA	9390	0	SER	F	69	65.105	51.273	69.462	1.00 43.11	F
MOTA	9391	N	asn	F	70	67.074	52.268	69.883	1.00 38.69	F
MOTA	9392	CA	ASN	F	70	67.037	52.001	71.317	1.00 38.12	F
ATOM	9393	CB	ASN	F	70	68.330	51.302	71.736	1.00 37.38	F
MOTA	9394	CG	ASN		70	68.629	50.087	70.882	1.00 39.74	F
ATOM	9395		ASN		70	67.715	49.421	70.415	1.00 44.47	F
MOTA	9396		ASN	F	70	69.911	49.786	70.683	1.00 41.63	F
MOTA	9397	C	ASN		70	66.812	53.180	72.250	1.00 41.52	F
MOTA	9398	0	ASN		70	66.785	53.006	73.471	1.00 46.38	F
MOTA	9399	N	PHE		71	66.643	54.377	71.713	1.00 40.71	F
ATOM	9400	CA	PHE		71	66.479	55.512	72.599	1.00 37.28	F
MOTA	9401	CB	PHE		71	67.773	56.326	72.645	1.00 29.09	F
MOTA	9402	CG	PHE		71	68.948	55.591	73.224	1.00 23.70	F
ATOM	9403		PHE		71	69.636	54.644	72.471	1.00 27.84	F
MOTA	9404		PHE		71	69.373	55.849	74.537	1.00 16.77	F
MOTA	9405	CEL	PHE	r'	71	70.750	53.953	73.031	1.00 36.93	F

ATOM	9406	CE2	PHE	F	71	70.469	55.177	75.101	1.00 19.07	F
ATOM	9407	cz	PHE	F	71	71.162	54.230	74.357	1.00 23.05	F
ATOM	9408	C	PHE	F	71	65.352	56.445	72.216	1.00 41.57	F
MOTA	9409	0	PHE		71	64.819	56.398	71.097	1.00 43.17	F
MOTA	9410	N	SER	F	72	64.980	57.280	73.178	1.00 39.92	F
ATOM	9411	CA	SER	F	72	63.967	58.305	72.973	1.00 45.02	F
ATOM	9412	CB	SER		72	62.679	58.011	73.749	1.00 46.23	F
MOTA	9413	OG	SER		72	62.892	58.094	75.144	1.00 54.10	F
ATOM	9414	C	SER		72	64.703	59.477	73.586	1.00 45.49	F
ATOM	9415	0	SER		72	65.364	59.326	74.617	1.00 45.76	F
ATOM	9416	N	GLY		73	64.641	60.641	72.969	1.00 45.34	F
ATOM	9417	CA	GLY		73	65.398	61.705	73.576	1.00 46.34	F
ATOM	9418	C	GLY		73	65.116	63.112	73.159	1.00 44.44	F
ATOM	9419	0	.GLY		73	64.289	63.387	72.279	1.00 42.38	F
ATOM ATOM	9420	N	THR		74	65.820	64.013	73.826	1.00 42.62	F
ATOM	9421 9422	CA CB	THR		74	65.664	65.416	73.535	1.00 46.94	. F
ATOM	9423	OGI	THR		74 74	65.047 65.981	66.199	74.745	1.00 45.06	F
ATOM	9424	CG2	THR		74	63.755	66.231 65.553	75.829	1.00 49.66	F
ATOM	9425	C	THR		74	67.013	66.020	75.208 73.200	1.00 35.87 1.00 44.87	P
ATOM	9426	Õ	THR		74	68.071	65.411	73.200	1.00 44.87	F F
ATOM	9427	N	VAL		75	66.955	67.215	72.629	1.00 46.10	F
ATOM	9428	CA	VAL		75	68.160	67.954	72.299	1.00 47.48	F
ATOM	9429	CB	VAL		75	68.310	68.207	70.759	1.00 48.87	F
ATOM	9430		VAL		75	67.087	68.967	70.200	1.00 41.65	F
ATOM	9431		VAL		75	69.599	68.971	70.498	1.00 38.69	F
ATOM	9432	С	VAL	F	75	68.057	69.282	73.031	1.00 46.89	F
MOTA	9433	0	VAL	F	75	67.070	70.015	72.881	1.00 41.30	·F
ATOM	9434	N	LYS	F	76	69.060	69.567	73.852	1.00 47.29	F
ATOM	9435	CA	LYS	F	76	69.077	70.820	74.581	1.00 50.34	F
MOTA	9436	CB	LYS	F	76	69.597	70.621	76.009	1.00 51.71	F
ATOM	9437	CG	LYS	F	76	69.270	71.788	76.933	1.00 55.24	F
MOTA	9438	CD	LYS	F	76	69.735	71.555	78.363	1.00 60.80	F
MOTA	9439	CE	LYS		76	69.274	72.695	79.284	1.00 63.97	F
ATOM	9440	NZ	LYS		76	69.701	72.497	80.706	1.00 68.67	F
ATOM	9441	C	LYS		76	69.973	71.813	73.843	1.00 51.42	F
ATOM	9442	0	LYS		76	71.199	71.697	73.870	1.00 50.94	F
ATOM	9443	N	TYR		77	69.348	72.785	73.183	1.00 49.81	F
MOTA	9444	CA	TYR		77	70.084	73.805	72.456	1.00 49.19	F
ATOM	9445	CB	TYR		77	69.556	73.963	71.036	1.00 40.66	F
MOTA	9446	CG	TYR		77	70.390	74.929	70.234	1.00 42.35	F
ATOM	9447	CD1	TYR		77	71.763	74.744	70.107	1.00 40.77	F
ATOM ATOM	9448 9449	CE1	TYR TYR		77 77	72.530	75.592	69.330	1.00 44.94	F
ATOM	9450	CE2	TYR	_	77	69.808 70.567	76.004 76.867	69.566	1.00 45.11	F
ATOM	9451	CZ	TYR		77	71.931	76.652	68.778 68.658	1.00 38.35	F
ATOM	9452	OH	TYR		77	72.700	77.449	67.825	1.00 46.15 1.00 47.81	F
ATOM	9453	C	TYR		77	70.032	75.180	73.099	1.00 47.81	F F
ATOM	9454	ō	TYR		77	69.024	75.880	72.973	1.00 54.64	F
ATOM	9455	N	SER		7.8	71.111	75.575	73.765	1.00 51.37	F
ATOM	9456	CA	SER		78	71.167	76.901	74.361	1.00 52.39	F
MOTA	9457	CB	SER		78	71.001	77.961	73.249	1.00 51.04	F
ATOM	9458	OG	SER		78	71.215	79.296	73.699	1.00 46.53	F
ATOM	9459	C	SER		78	70.098	77.095	75.429	1.00 55.65	F
ATOM	9460	0	SER		78	69.308	78.036	75.361	1.00 58.01	F
ATOM	9461	N	GLY		79	70.055	76.204	76.410	1.00 58.16	F
MOTA	9462	CA	GLY		79	69.067	76.364	77.463	1.00 62.32	F
MOTA	9463	C	GLY		79	67.700	75.728	77.271	1.00 63.66	F

MOTA	9464	0	GLY	F	79	67.064	75.372	78.257	1.00 65.24	F
ATOM	9465	N	SER		80	67.239	75.594	76.027	1.00 63.68	F
MOTA	9466	CA	SER	F	80	65.935	74.984	75.749	1.00 63.15	F
MOTA	9467	CB	SER	F	80	65.156	75.841	74.762	1.00 60.98	F
MOTA	9468	OG	SER	F	80	64.840	77.081	75.354	1.00 68.24	F
MOTA	9469	С	SER	F	80	66.041	73.558	75.203	1.00 63.15	F
MOTA	9470	0	SER	F	80	67.094	73.156	74.697	1.00 62.36	· F
ATOM	9471	N	SER	F	81	64.949	72.796	75.302	1.00 60.19	F
MOTA	9472	CA	SER	F	81	64.947	71.417	74.817	1.00 54.17	F
ATOM	9473	CB	SER	F	81	64.682	70.428	75.958	1.00 56.00	F
MOTA	9474	OG	SER	F	81	65.892	69.881	76.466	1.00 55.39	F
MOTA	9475	C	SER	F	81	63.950	71.187	73.706	1.00 50.61	F
MOTA	9476	0	SER	F	81	62.938	71.860	73.601	1.00 47.11	F
MOTA	9477	N	TYR	F	82	64.264	70.231	72.850	1.00 52.61	F
ATOM	9478	CA	TYR	F	82	63.400	69.919	71.728	1.00 51.05	F
MOTA	9479	CB	TYR	F	82	63.838	70.695	70.469	1.00 52.08	F
MOTA	9480	CG	TYR		82	64.098	72.175	70.692	1.00 54.57	F
ATOM	9481	CD1			82	65.221	72.610	71.399	1.00 51.96	F
ATOM	9482	CEI			82	65.431	73.967	71.666	1.00 55.73	F
ATOM	9483		TYR	_	82	63.192	73.140	70.243	1.00 59.64	F
MOTA	9484	CE2	TYR		82	63.393	74.508	70.501	1.00 55.89	F
ATOM	9485	CZ	TYR		82	64.513	74.912	71.214	1.00 59.54	F
MOTA	9486	OH	TYR		82	64.713	76.254	71.480	1.00 63.13	F
ATOM	9487	C	TYR		82	63.489	68.423	71.461	1.00 48.76	F
ATOM	9488	0	TYR		82	64.437	67.741	71.878	1.00 49.60	F
ATOM	9489	N	PRO		83	62.499	67.894	70.755	1.00 43.46	F
MOTA	9490 9491	CD	PRO	_	83	61.289	68.612	70.346	1.00 40.53	F
ATOM ATOM	9491	CA CB	PRO PRO		83	62.415	66.480	70.400	1.00 44.18	F
MOTA	9493	CG	PRO		83 83	61.075 60.296	66.388 67.514	69.691 70.289	1.00 42.13	F F
ATOM	9494	C.	PRO		83	63.557	66.061	69.486	1.00 44.41 1.00 45.02	F
ATOM	9495	Ö	PRO		83	63.829	66.726	68.484	1.00 45.02	F
ATOM	9496	N	PHE		84	64.224	64.960	69.815	1.00 47.21	F
ATOM	9497	CA	PHE		84	65.326	64.466	68.977	1.00 44.64	F
ATOM	9498	CB	PHE		84	66.660	64.592	69.704	1.00 44.94	F
ATOM	9499	CG	PHE		84	67.822	64.033	68.935	1.00 42.64	F
MOTA	9500	CD1	PHE	F	84	68.389	64.749	67.888	1.00 40.91	F
MOTA	9501	CD2	PHE	F	84	68.337	62.770	69.239	1.00 39.71	F
ATOM	9502	CEL	PHE	F	84	69.454	64.213	67.155	1.00 40.95	F
MOTA	9503	CE2	PHE	F	84	69.401	62.232	68.508	1.00 38.02	F
MOTA	9504	CZ	PHE	F	84	69.959	62.958	67.466	1.00 34.23	F
MOTA	9505	С	PHE	F	84	65.062	62.996	68.656	1.00 45.21	F
ATOM	9506	0	PHE	F	84	64.875	62.177	69.567	1.00 48.91	F
MOTA	9507	N	PRO		85	65.090	62.624	67.363	1.00 44.00	F
MOTA	9508	CD	PRO	F	85	64.852	61.212	67.011	1.00 39.93	F
MOTA	9509	CA	PRO		85	65.319	63.415	66,146	1.00 43.11	· F
MOTA	9510	CB	PRO		85	64.855	62.475	65.044	1.00 39.52	F
MOTA	9511	CG	PRO		85	65.324	61.149	65.569	1.00 37.09	F
MOTA	9512	C	PRO		85	64.560	64.721	66.168	1.00 42.70	F
ATOM	9513	0	PRO		85	63.465	64.777	66.710	1.00 45.67	F
ATOM	9514	N	THR		86	65.135	65.769	65.591	1.00 40.24	F
ATOM	9515	CA.	THR		86	64.482	67.065	65.601	1.00 40.17	F
ATOM	9516	CB	THR		86	65.469	68.168	65.273	1.00 37.73	F
ATOM	9517		THR		86	65.892	68.032	63.913	1.00 34.54	F
ATOM ATOM	9518	CG2			86 86	66.672 63.347	68.100	66.193	1.00 38.84	F
MOTA	9519	C	THR		86 86		67.120	64.605	1.00 44.75	F
ATOM	9520 9521	И О	THR		86 87	63.294 62.446	66.317 68.078	63.677 64.796	1.00 45.99	F
LT OIL	2247	7.4	THR	E,	0 /	02.440	90.078	04 - 130	1.00 48.99	Ľ

This Page is Inserted by IFW Indexing and Scanning Operations and is not part of the Official Record

BEST AVAILABLE IMAGES

Defective images within this document are accurate representations of the original documents submitted by the applicant.

Defects in the images include but are not limited to the items checked:

☑ BLACK BORDERS
☐ IMAGE CUT OFF AT TOP, BOTTOM OR SIDES
☐ FADED TEXT OR DRAWING
☐ BLURRED OR ILLEGIBLE TEXT OR DRAWING
☐ SKEWED/SLANTED IMAGES
☐ COLOR OR BLACK AND WHITE PHOTOGRAPHS
☐ GRAY SCALE DOCUMENTS
☐ LINES OR MARKS ON ORIGINAL DOCUMENT
☐ REFERENCE(S) OR EXHIBIT(S) SUBMITTED ARE POOR QUALITY
□ OTHER:

IMAGES ARE BEST AVAILABLE COPY.

As rescanning these documents will not correct the image problems checked, please do not report these problems to the IFW Image Problem Mailbox.